

Supporting Information

Facial Synthesis and Bioevaluation of Well-Defined OEGylated Betulinic Acid-Cyclodextrin Conjugates for Inhibition of Influenza Entry

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¹³ C NMR of compound 86	S65
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1. Figure S1.

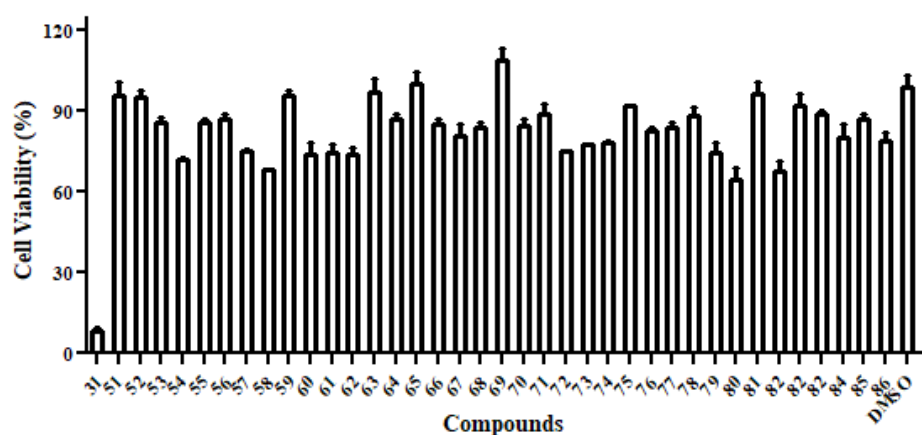


Figure S1. Cytotoxicity of multivalent BA-CD conjugates to MDCK cells. The cell viability of MDCK cells was analyzed at 36 h of incubation in the presence of BA (**31**) and its CD conjugates **51-86** at concentration of 100 μM . The CellTiter-Glo Luminescent cell viability assay kit was used. 1% DMSO acted as negative control. Error bars indicate the mean \pm SD of three independent experiments.

2. Figure S2.

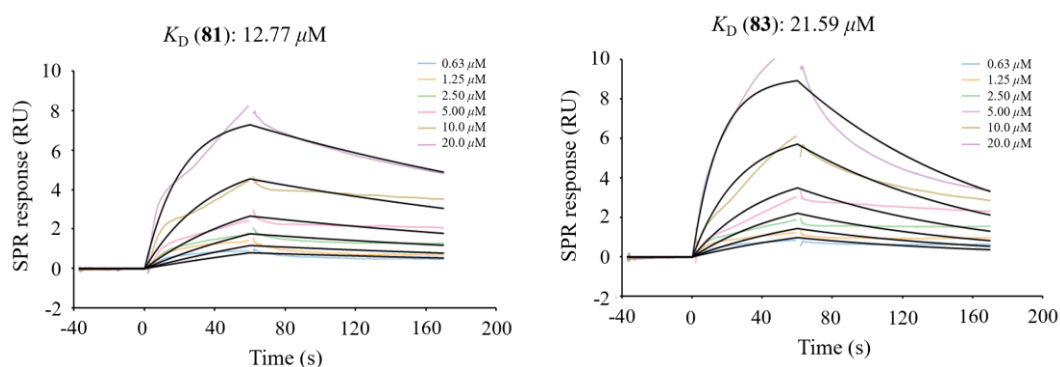
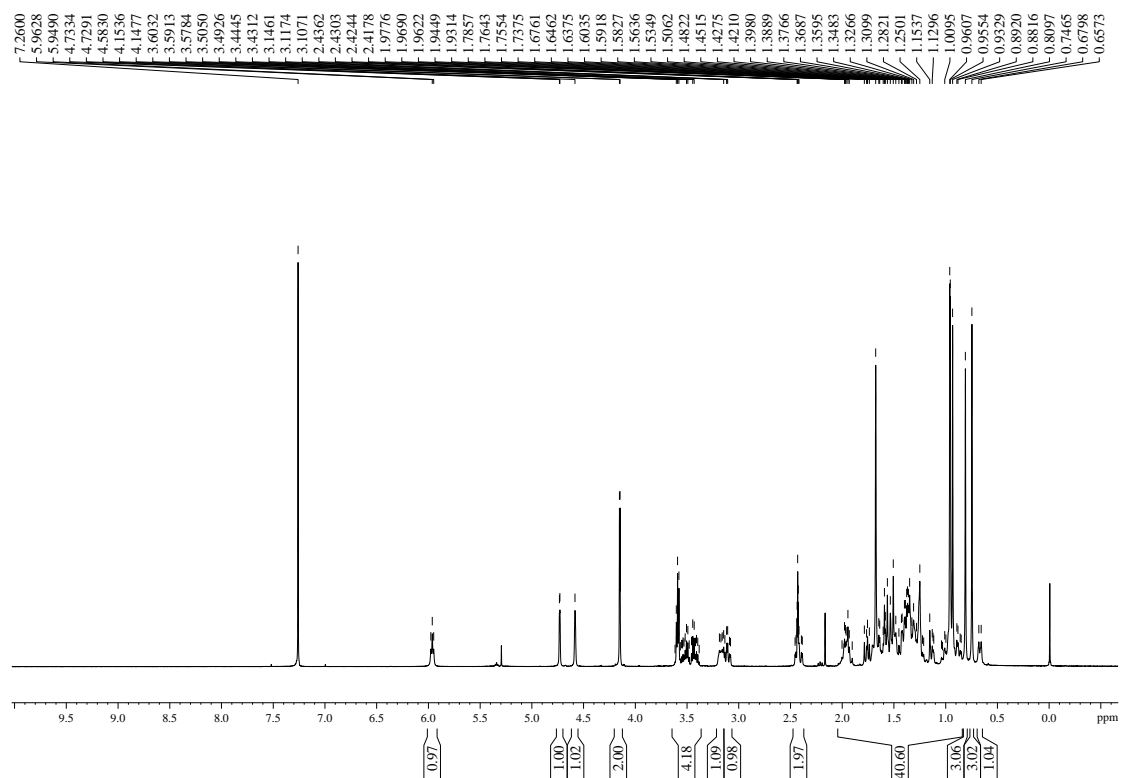


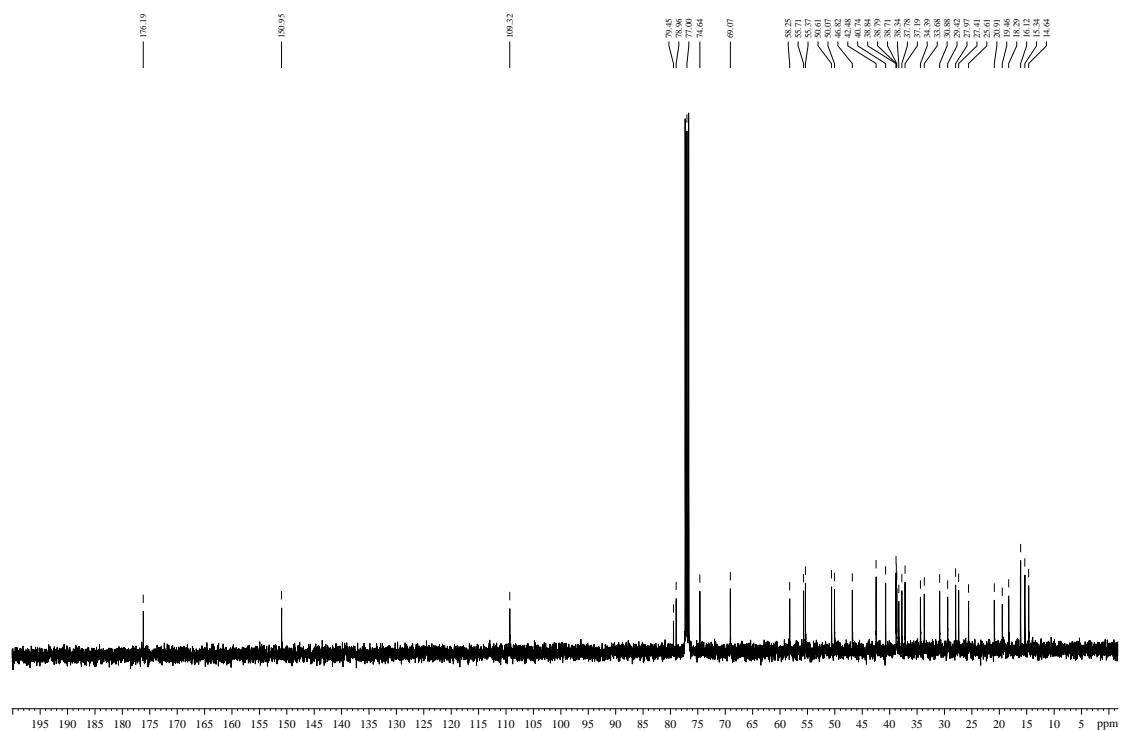
Figure S2. Binding sensorgrams for conjugates **81** and **83** interaction with influenza HA protein. The HA protein was immobilized on a CM5 sensor chip by the standard amine-coupling procedure. Different concentrations of conjugates **81** and **83** were flowed over the chip surface for a contact time of 60 s and a dissociation time of 180 s, respectively. K_D values were labeled in the graphs.

3. Selected NMR, HRMS and MALDI-TOF spectra

^1H NMR of compound **34**

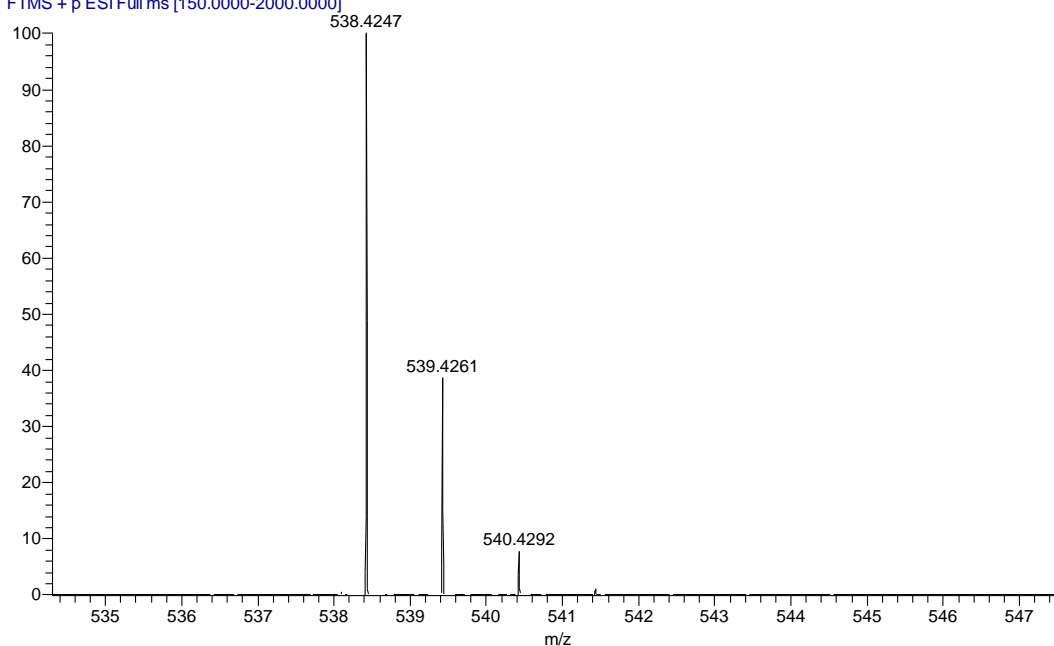


^{13}C NMR of compound **34**

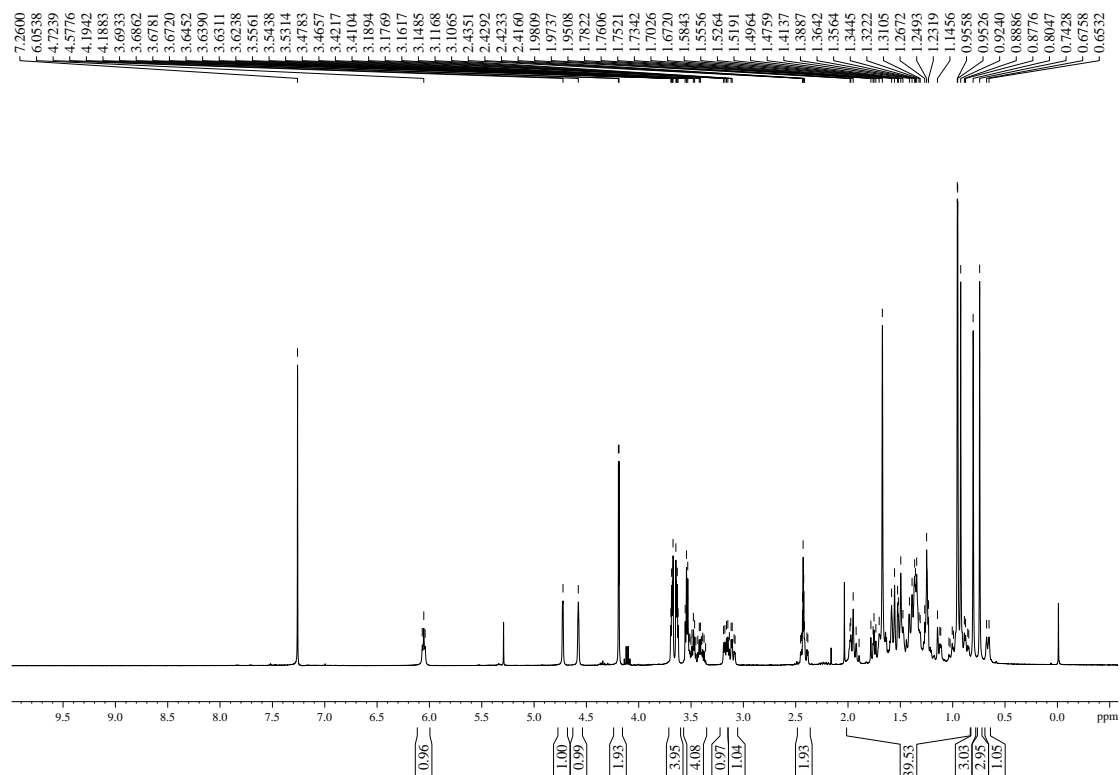


HRMS of compound **34**

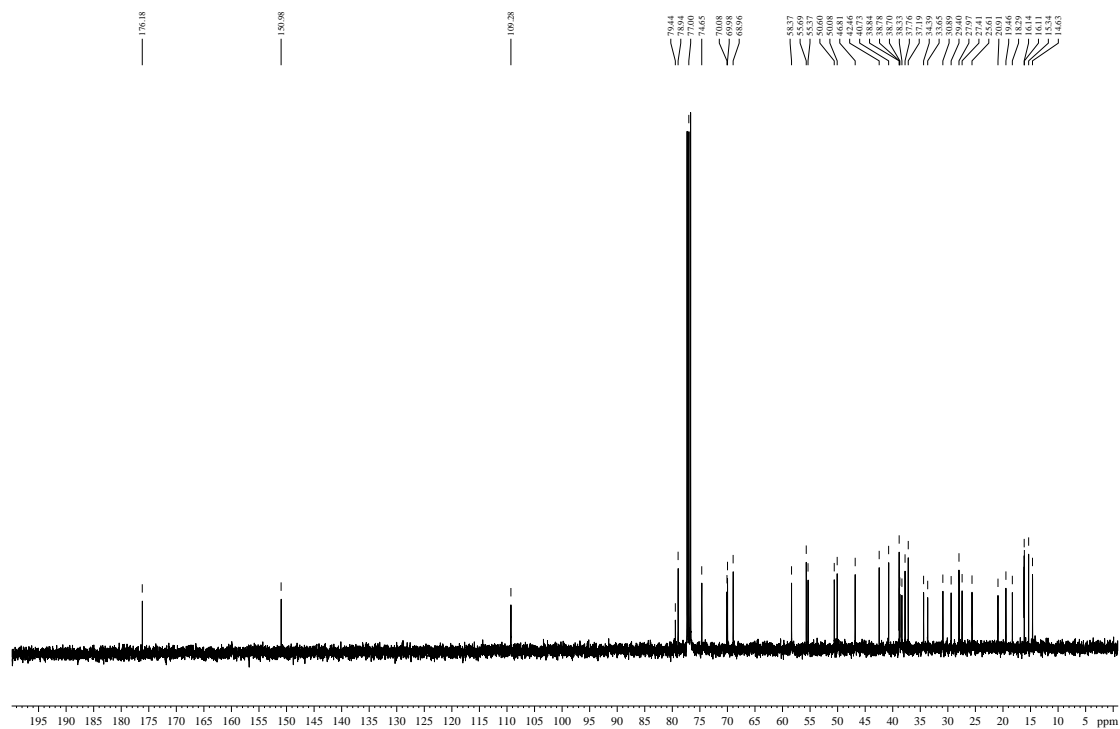
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T: FTMS + p ESI Full ms [150.0000-2000.0000]



^1H NMR of compound **35**

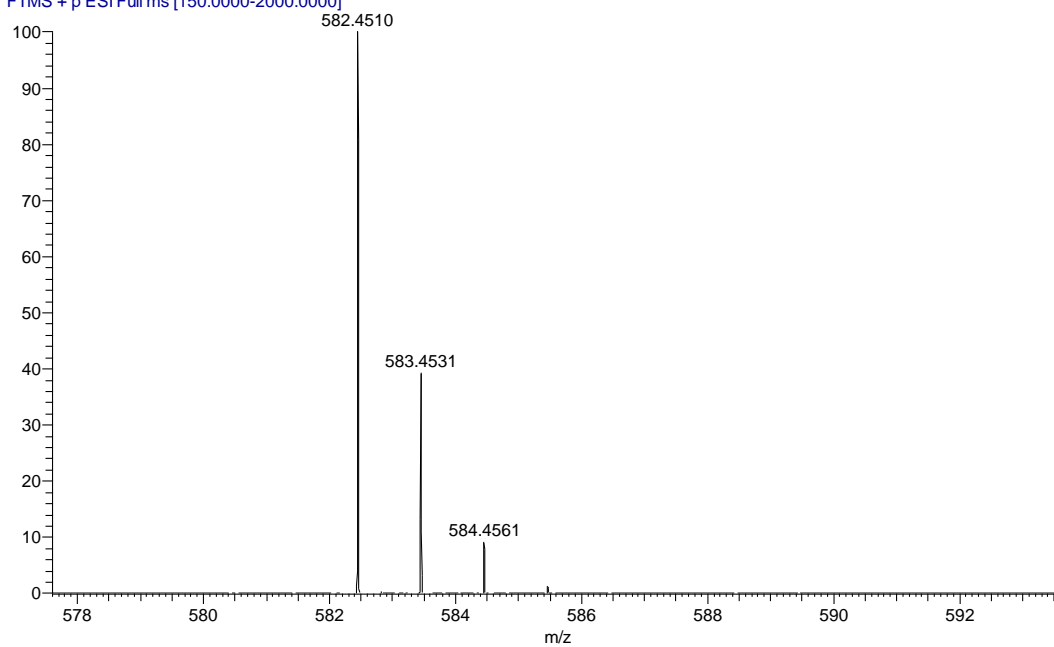


^{13}C NMR of compound **35**

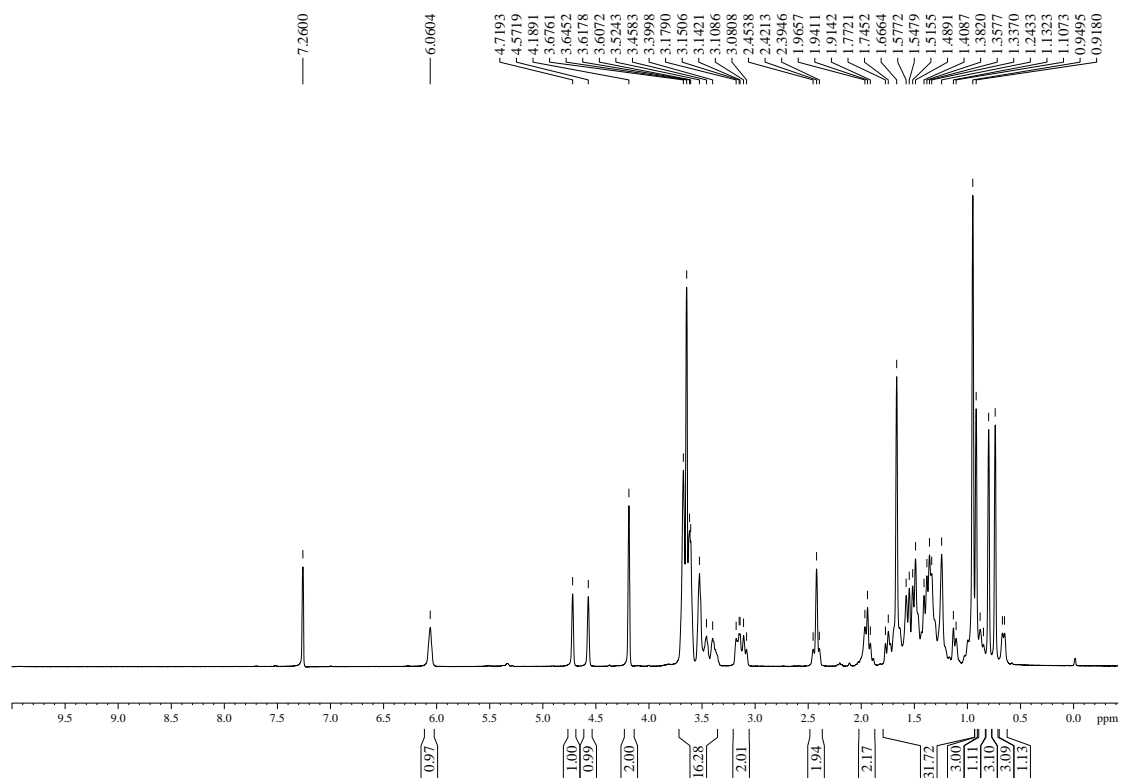


HRMS of compound **35**

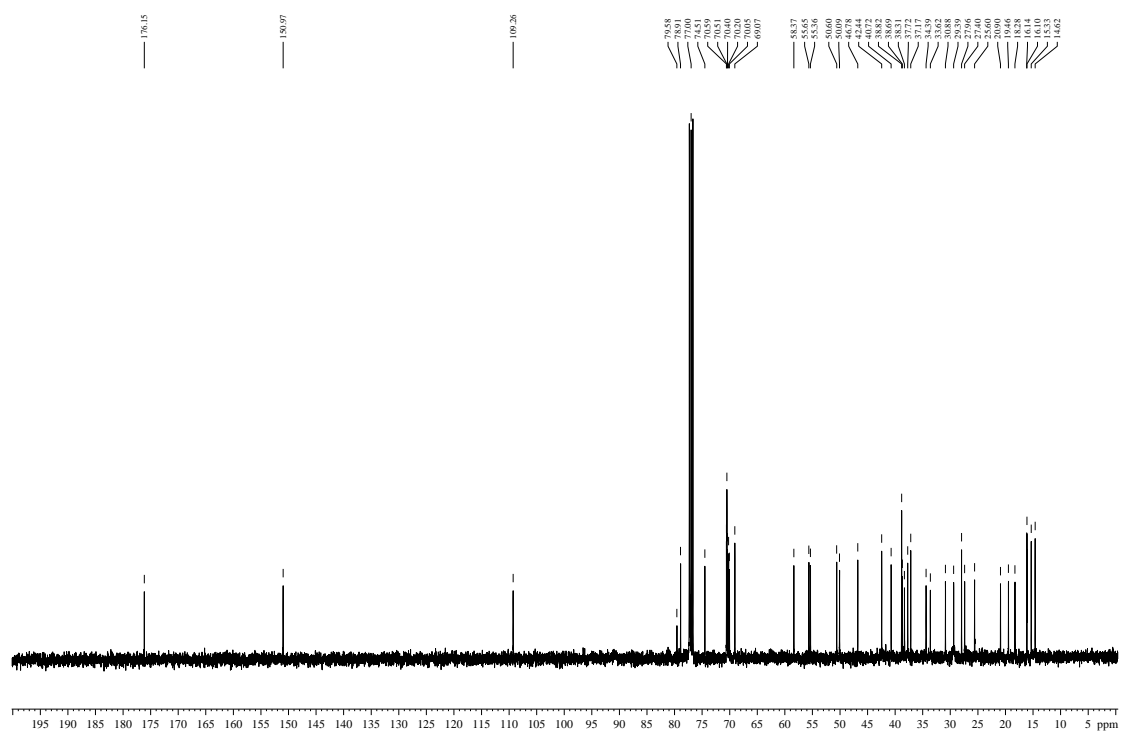
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¹H NMR of compound **36**



¹³C NMR of compound **36**



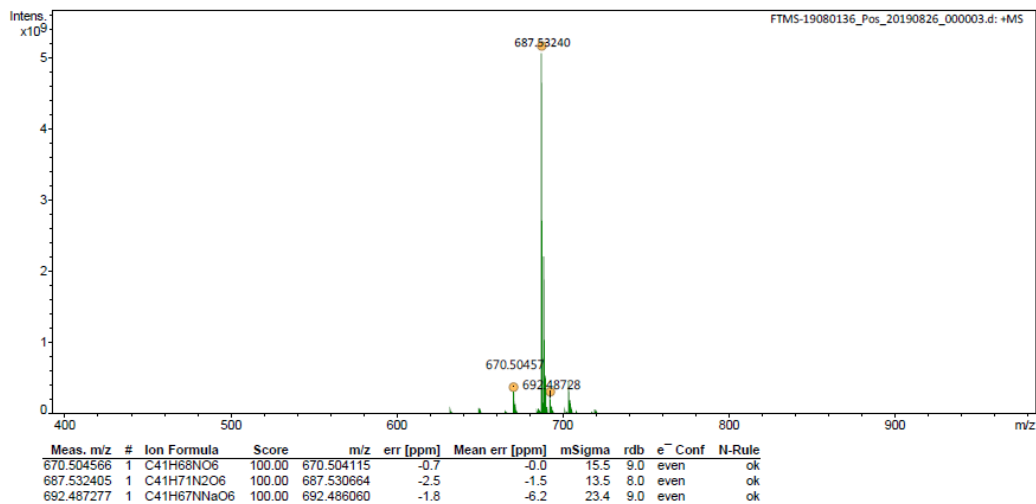
HRMS of compound **36**

Peking University Mass Spectrometry Sample Analysis Report

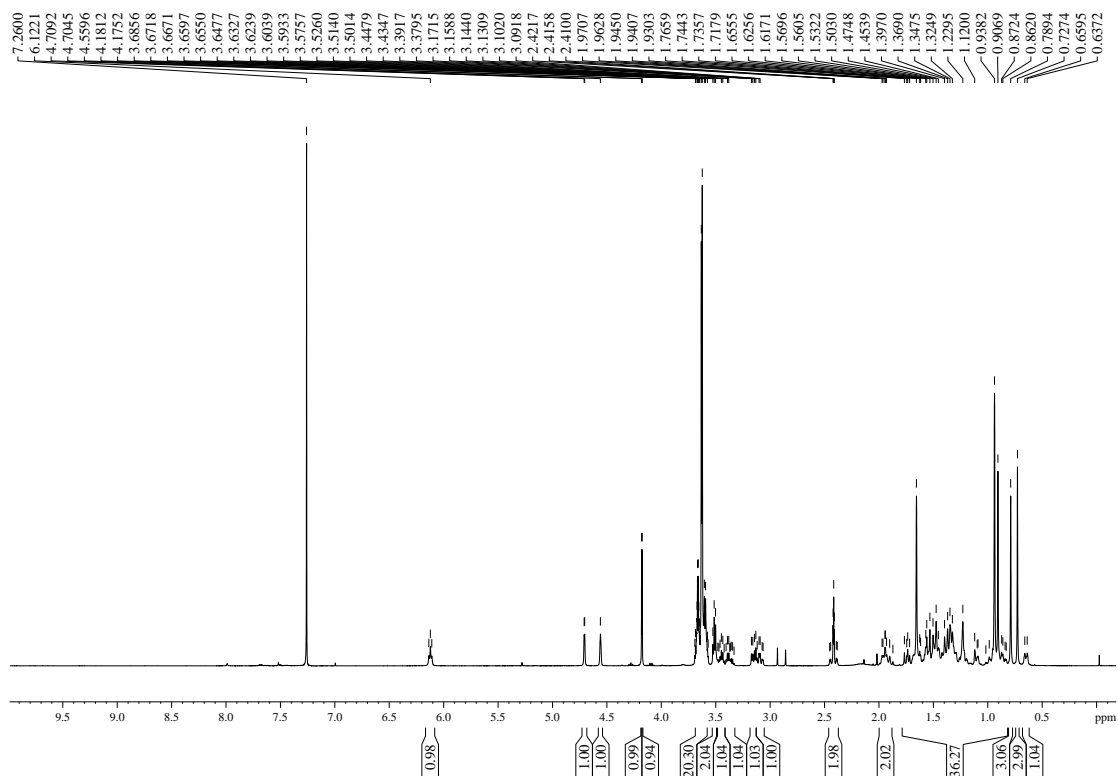
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Sample CYY-1-96
Comment

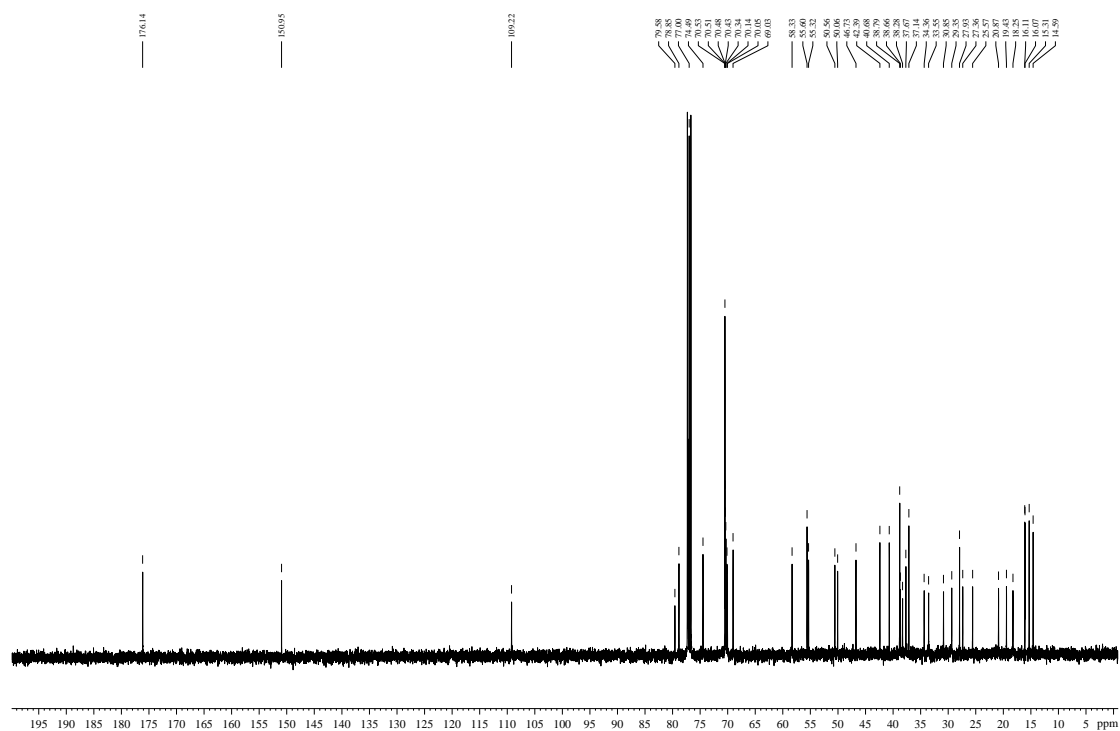
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Instrument Bruker Solarix XR FTMS
Operator Peking University



¹H NMR of compound **37**



¹³C NMR of compound **37**



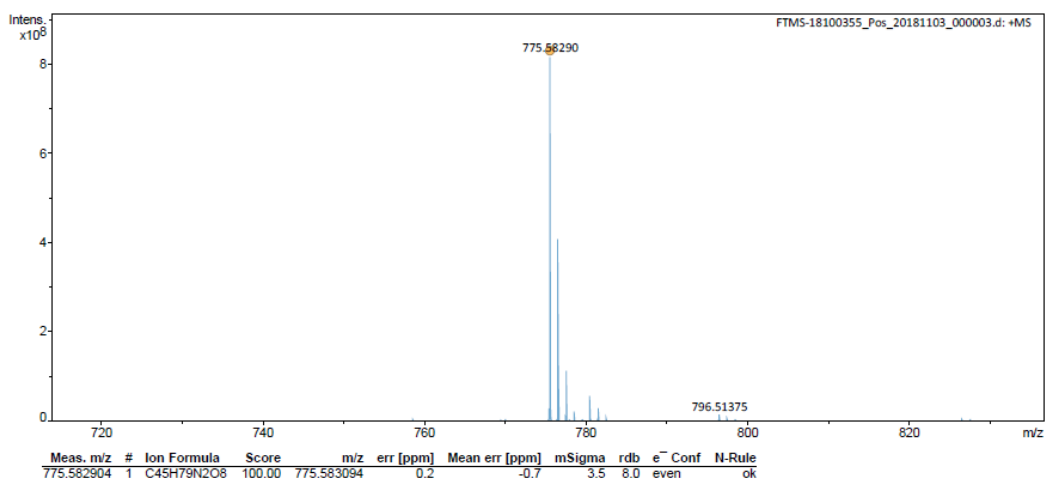
HRMS of compound **37**

Peking University Mass Spectrometry Sample Analysis Report

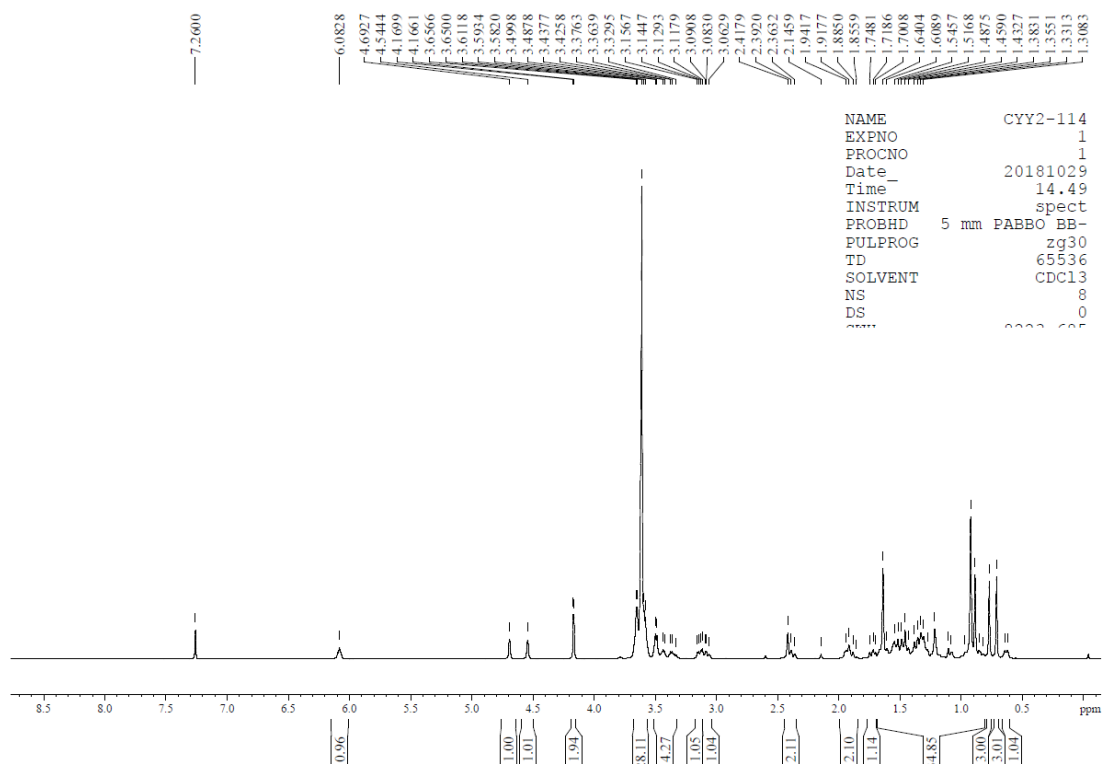
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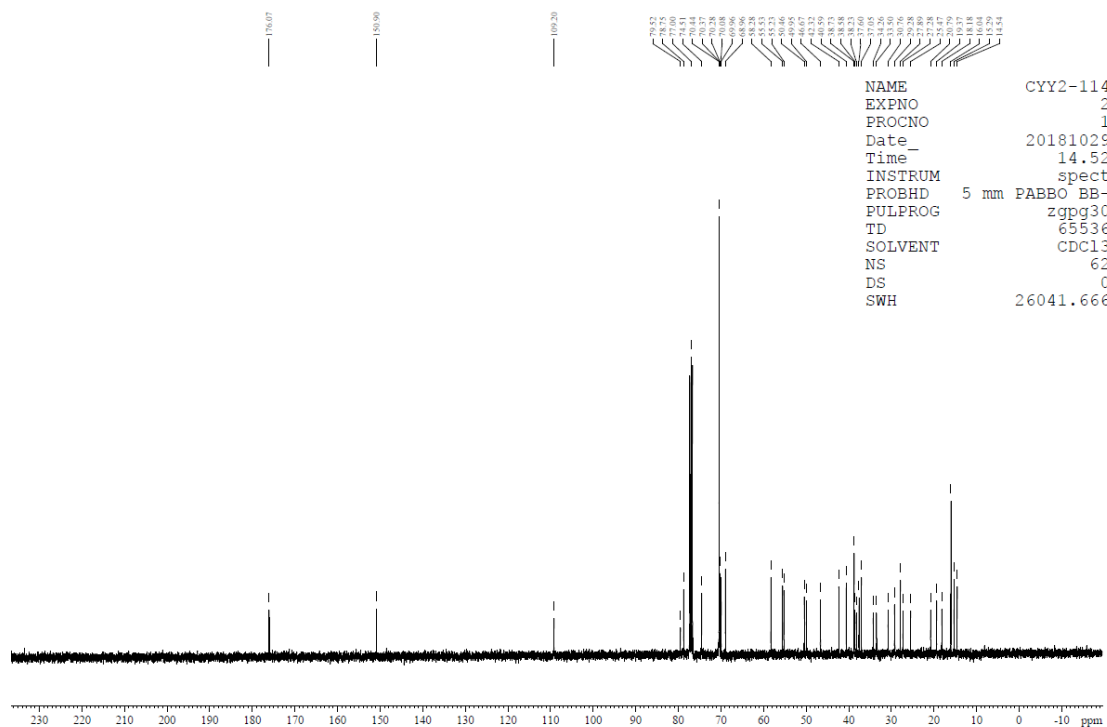
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Instrument Bruker Solarix XR FTMS
Operator Peking University



¹H NMR of compound **38**



¹³C NMR of compound **38**



HRMS of compound **38**

Peking University Mass Spectrometry Sample Analysis Report

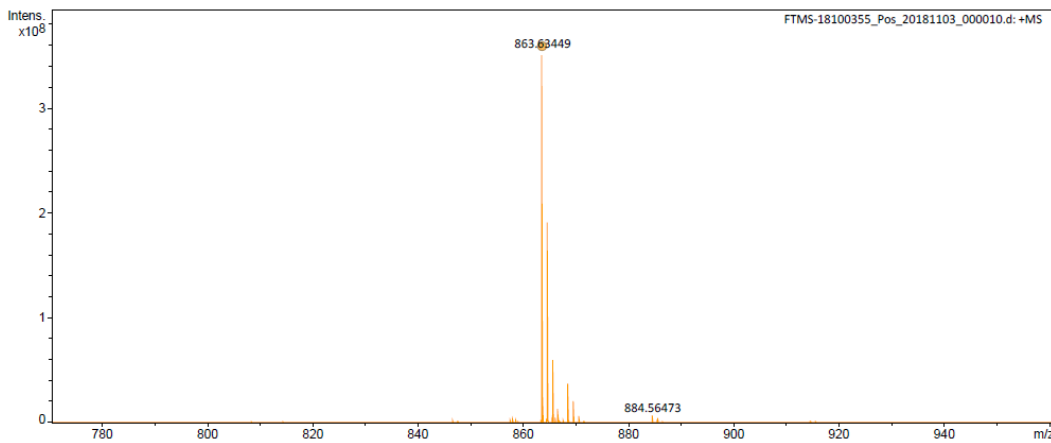
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Sample
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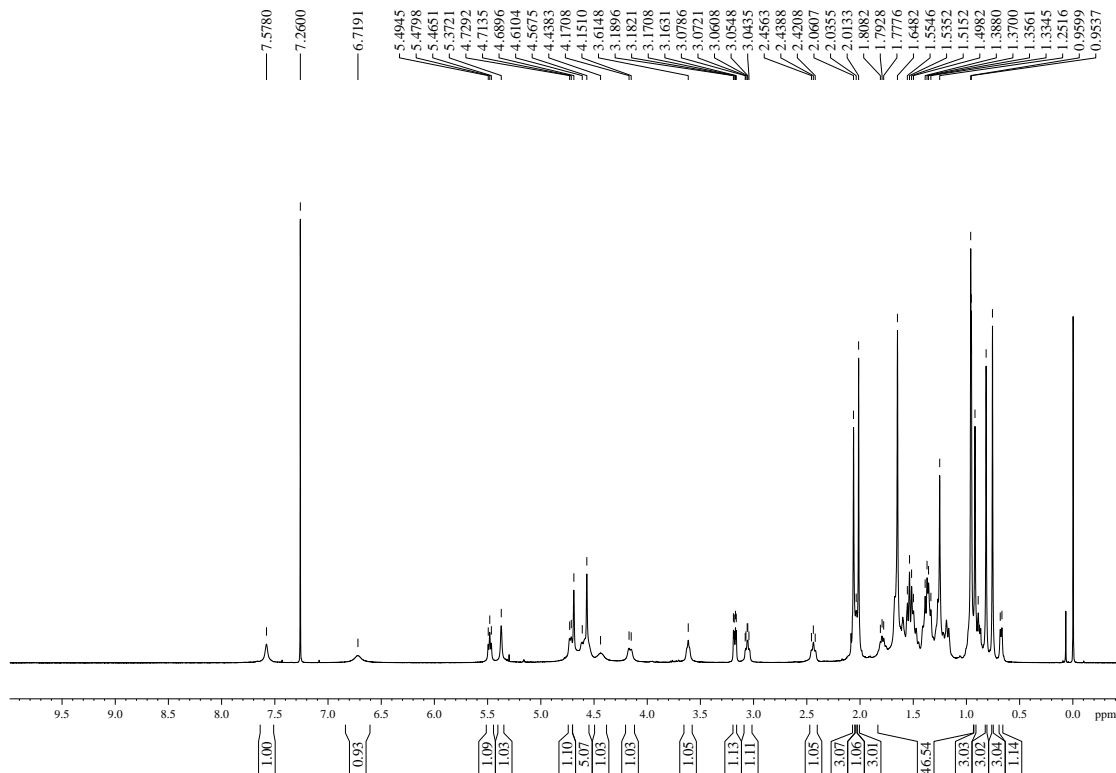
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Bruker Solarix XR FTMS
Peking University

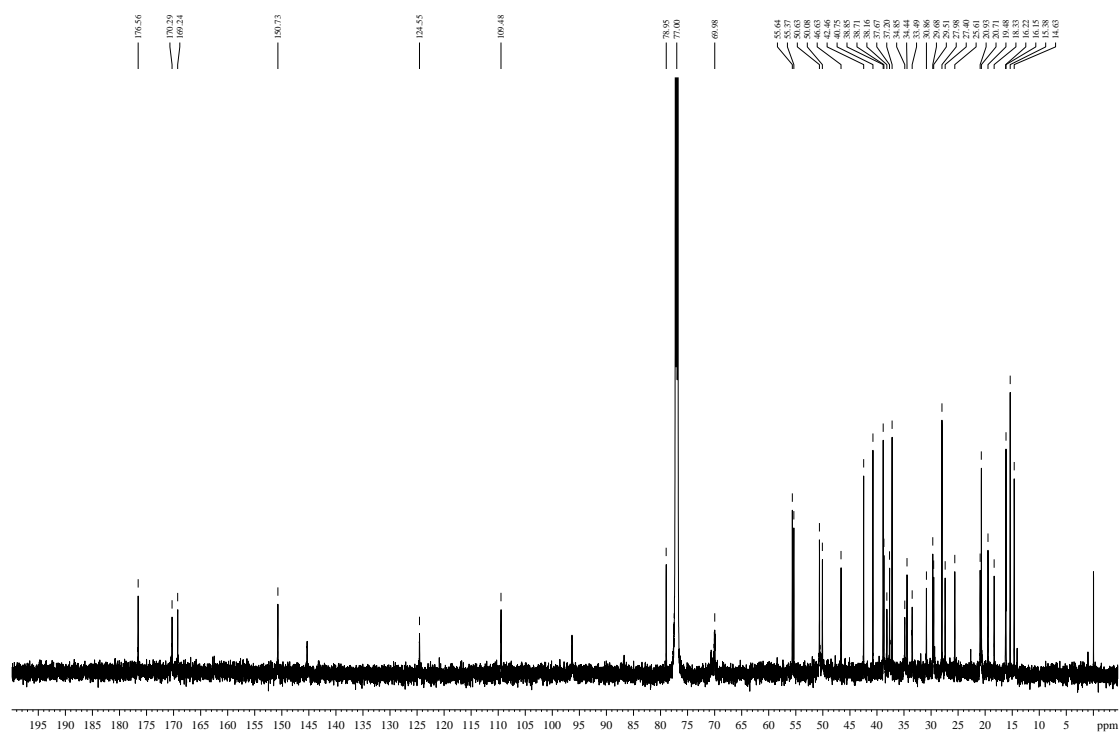


Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
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¹H NMR of compound **51**

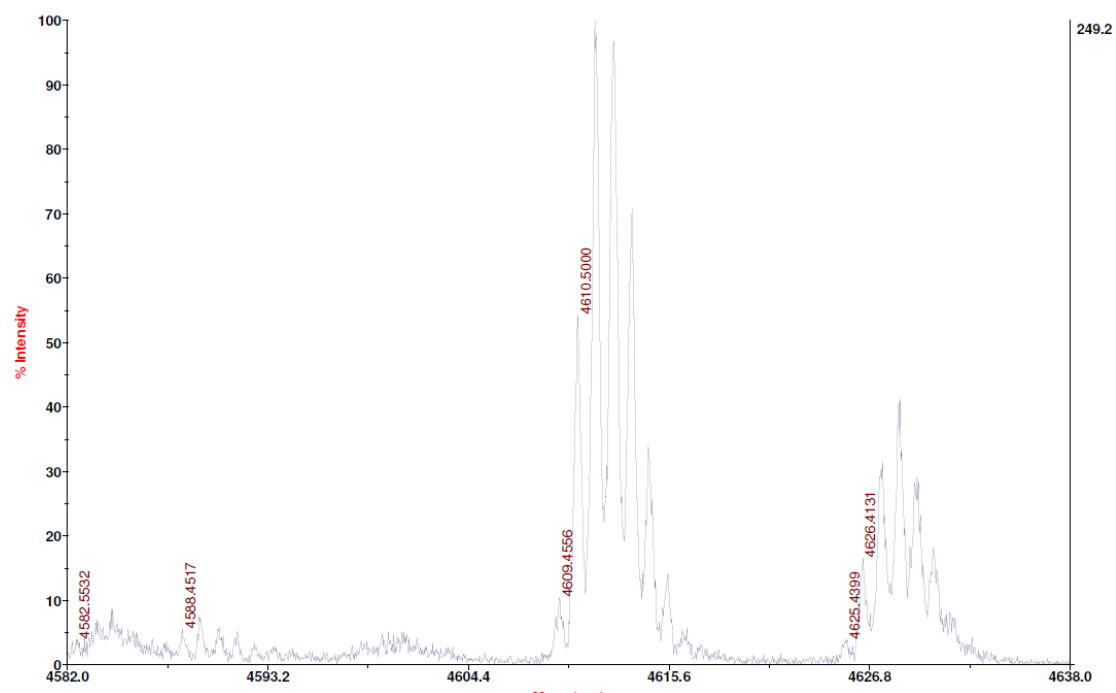


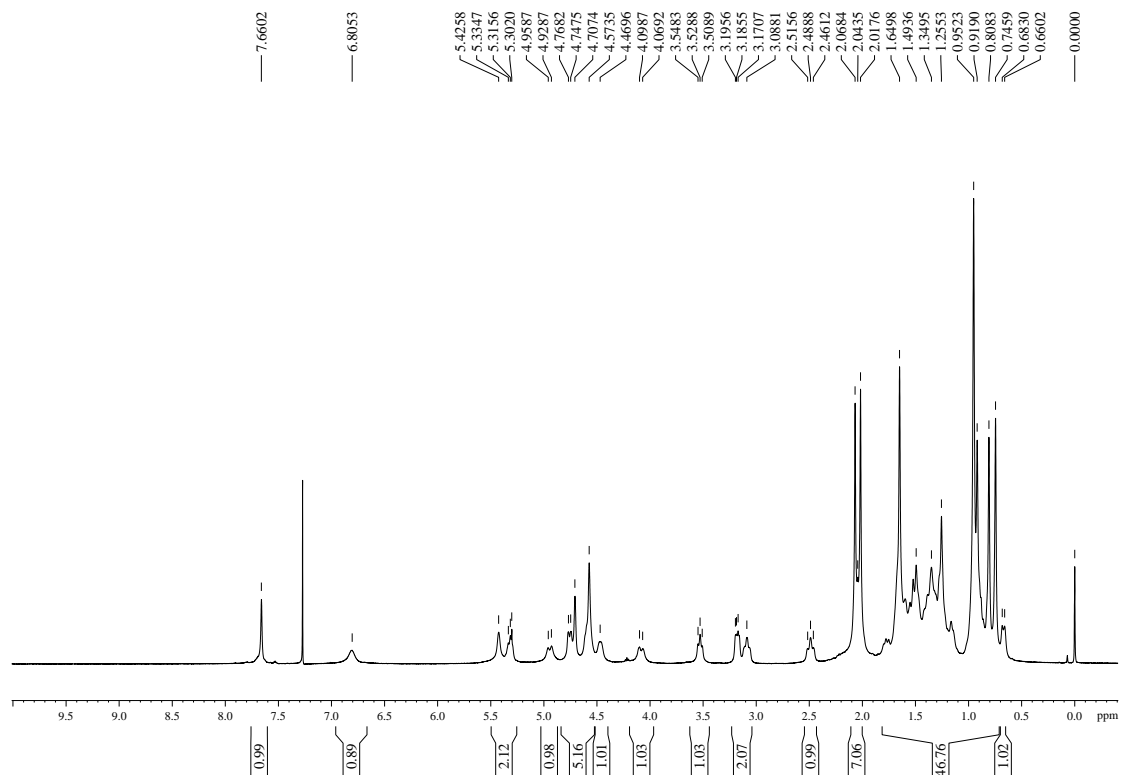
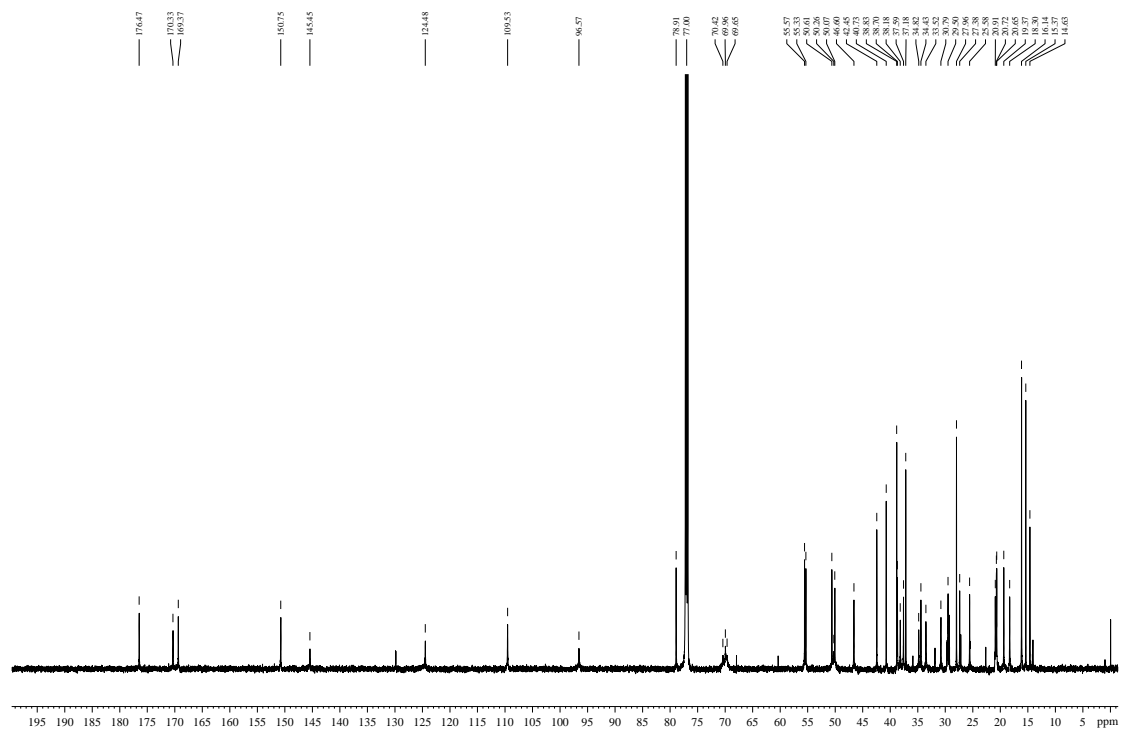
¹³C NMR of compound **51**



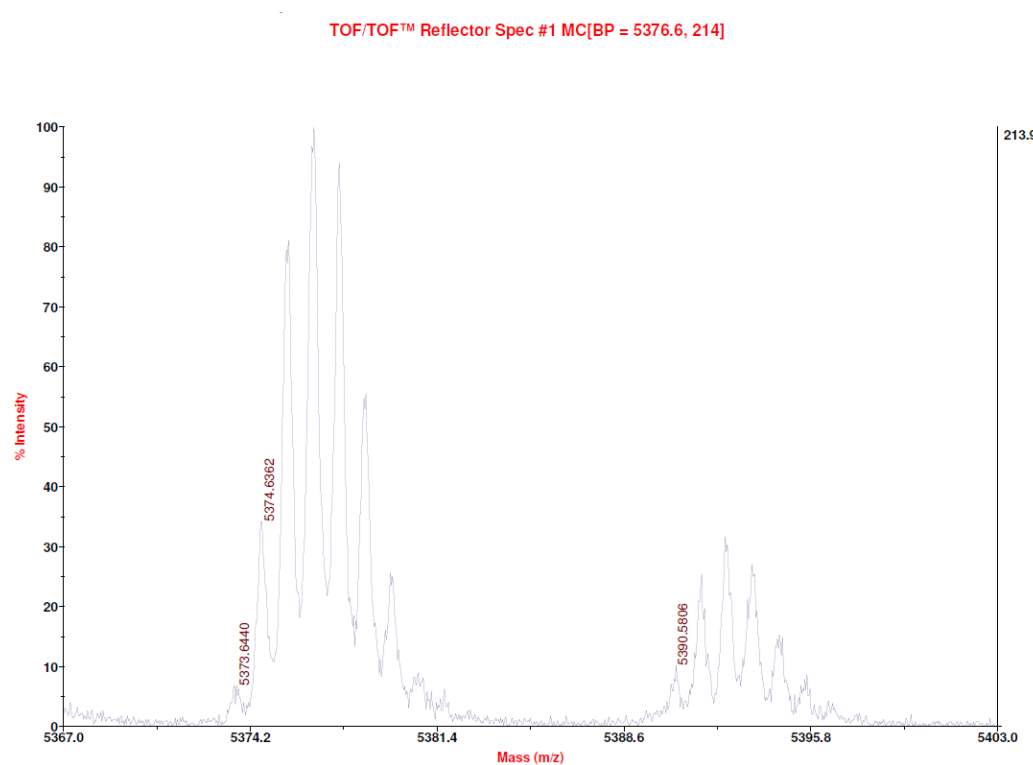
MALDI-TOF of compound **51**

TOF/TOF™ Reflector Spec #1 MC[BP = 4611.5, 249]

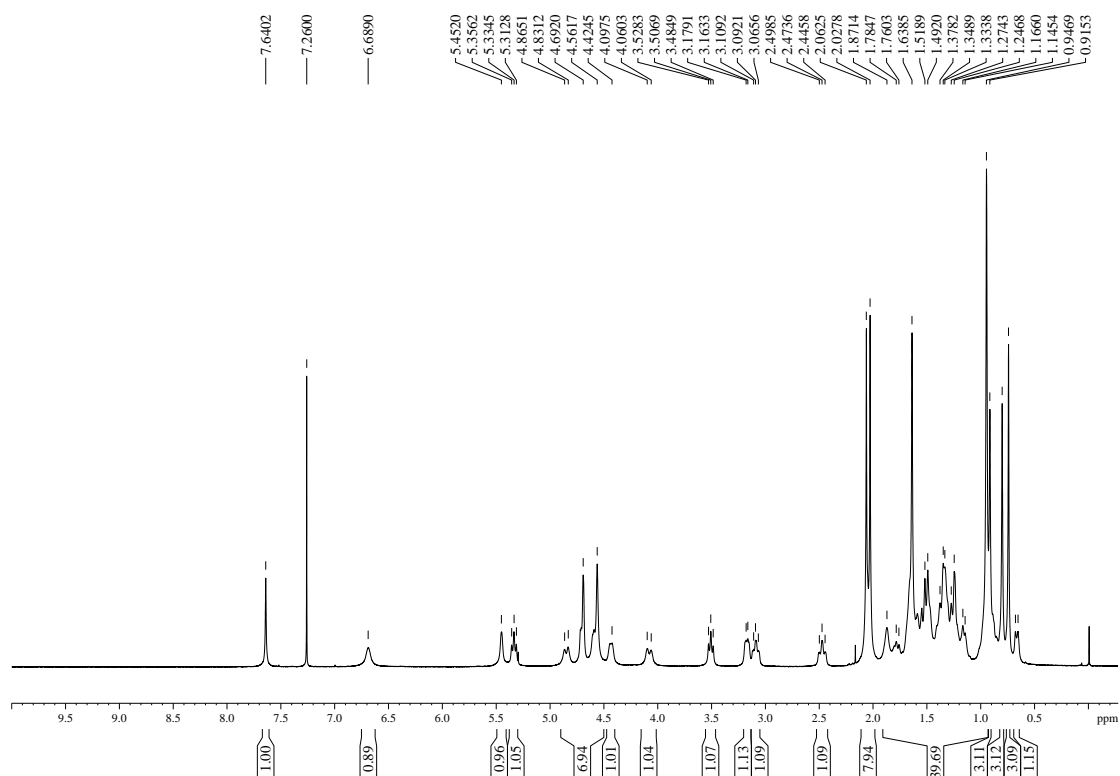


¹H NMR of compound **52** ^{13}C NMR of compound **52**

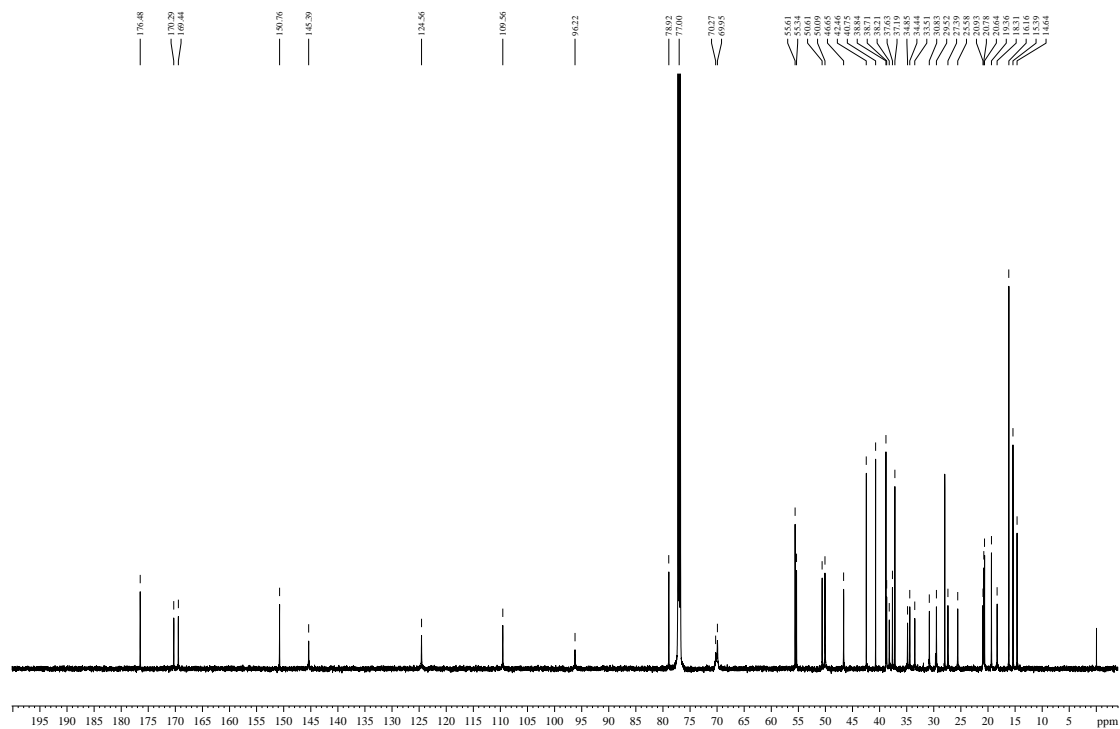
MALDI-TOF of compound **52**



^1H NMR of compound **53**

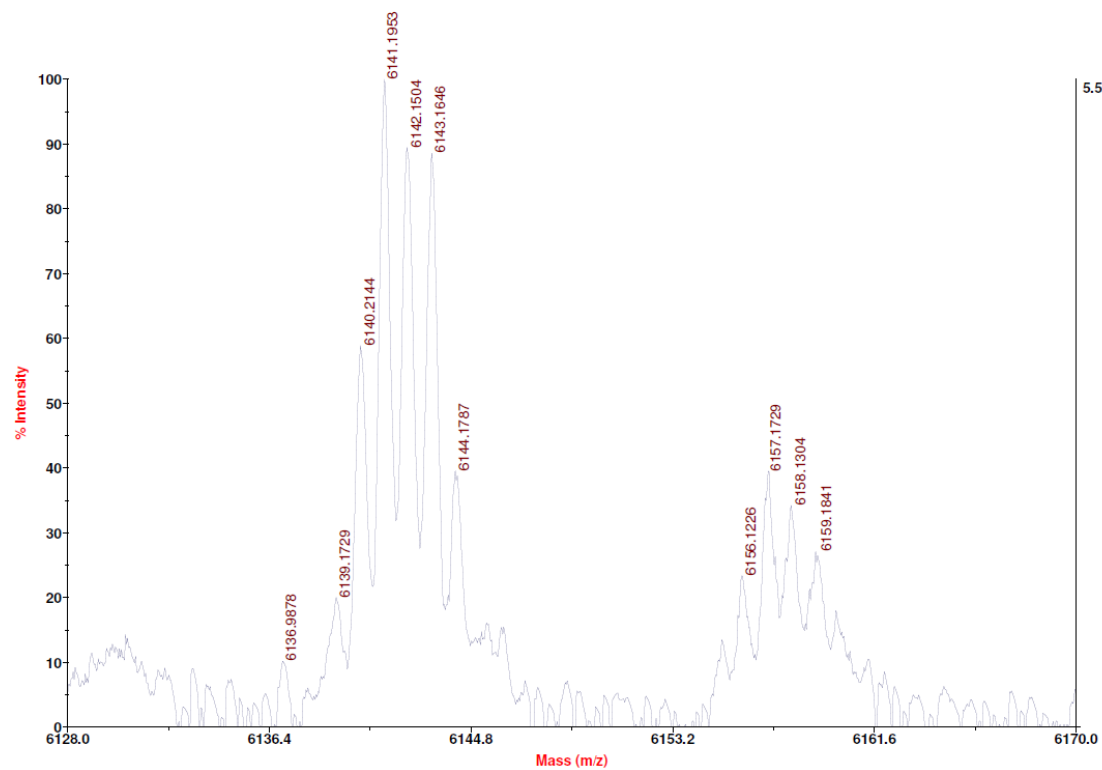


^{13}C NMR of compound **53**

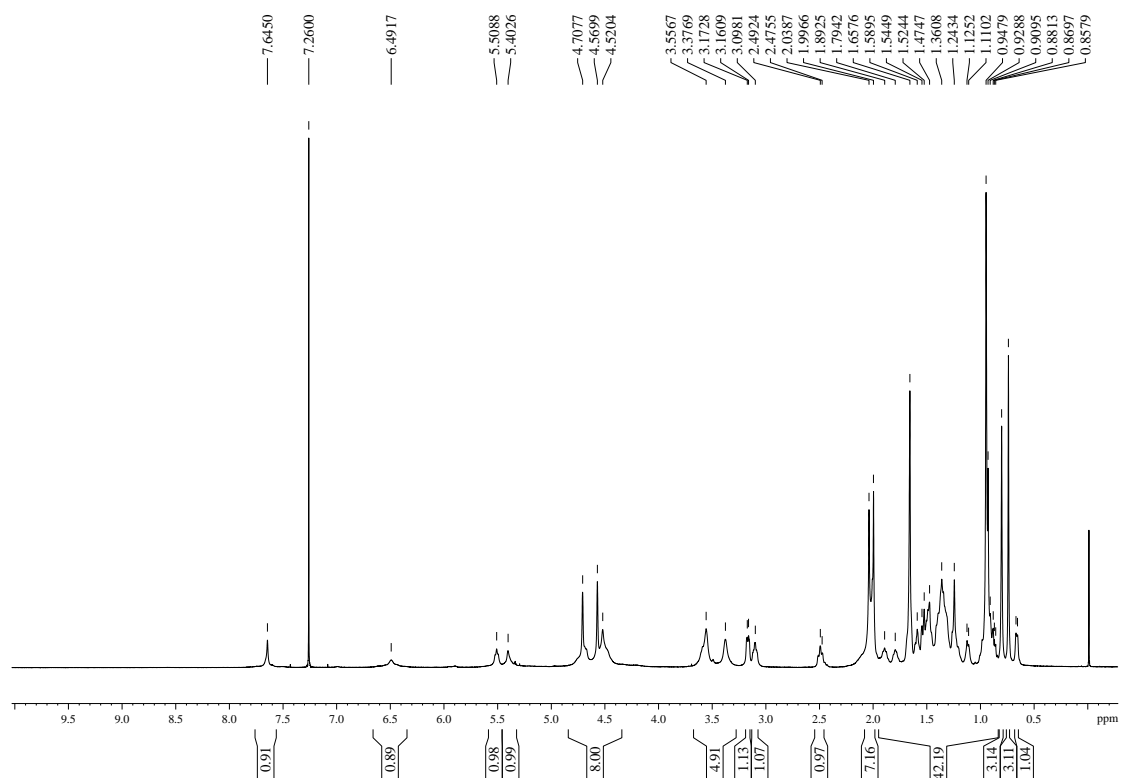


MALDI-TOF of compound **53**

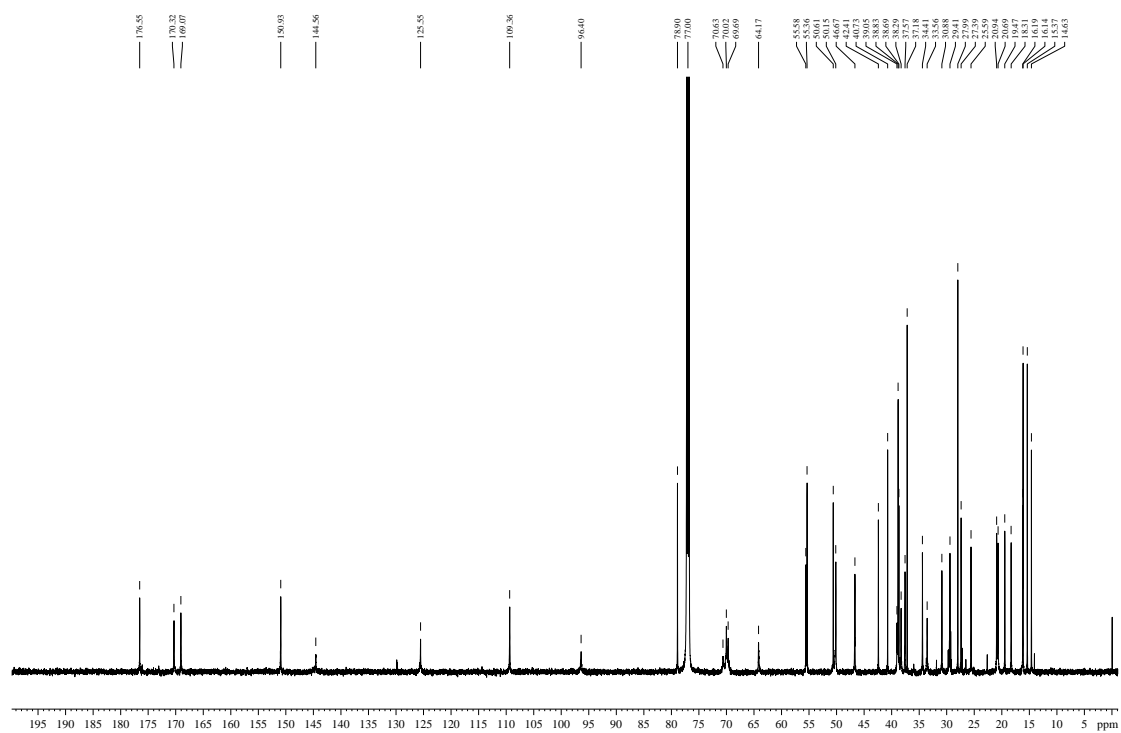
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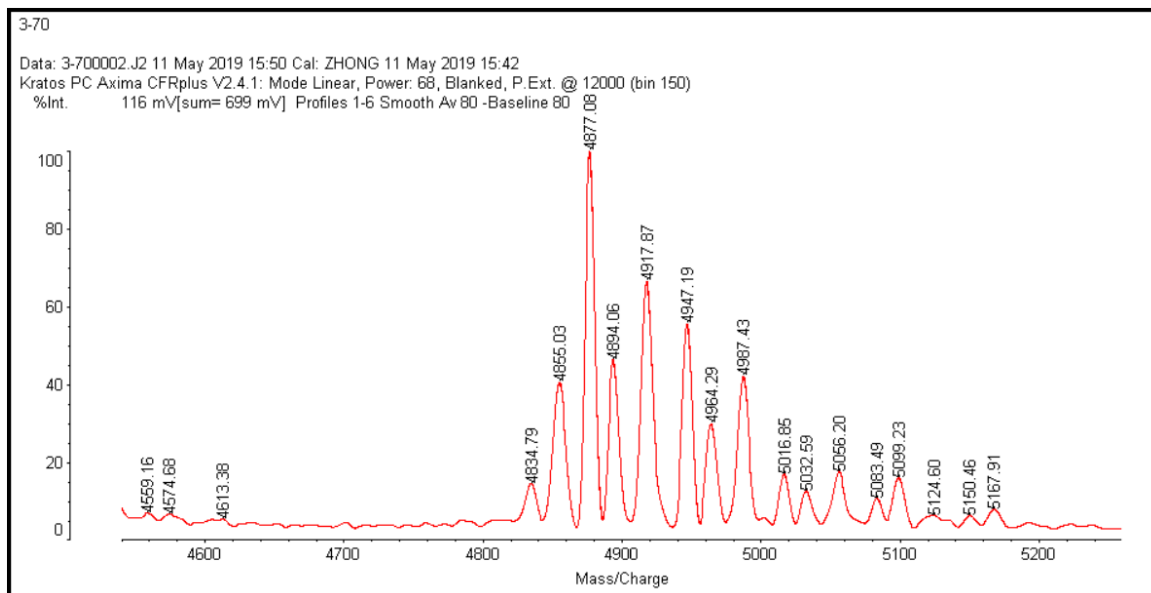
¹H NMR of compound **54**



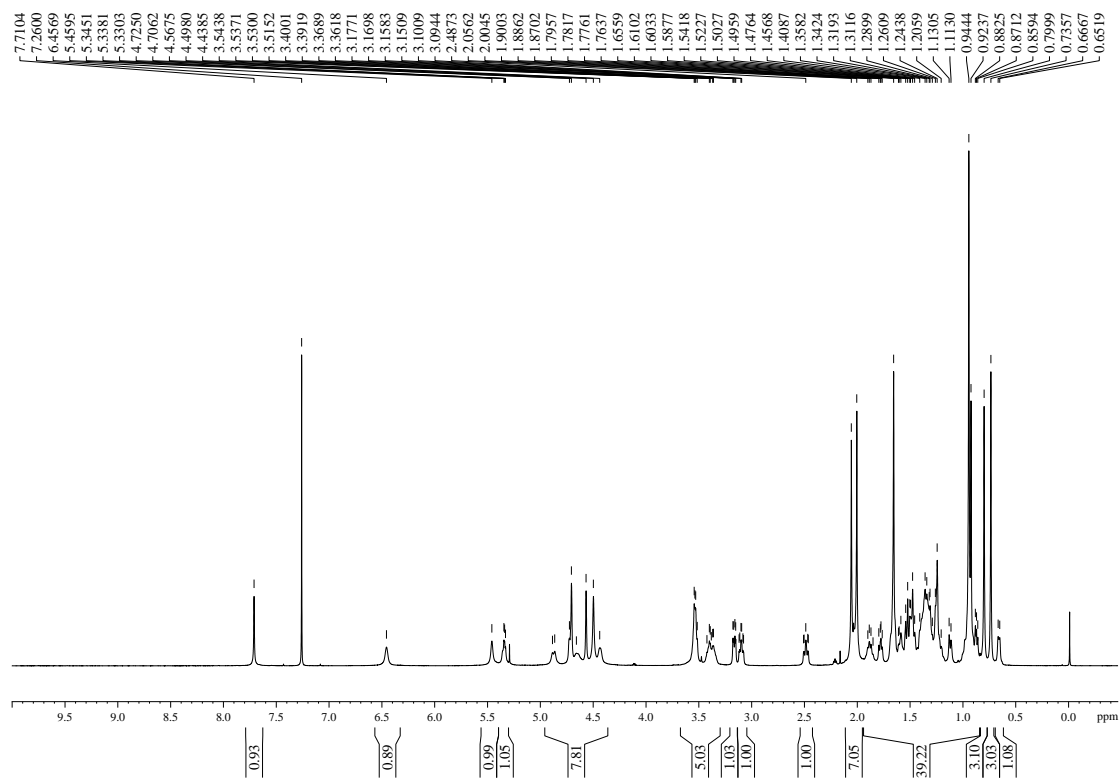
¹³C NMR of compound **54**



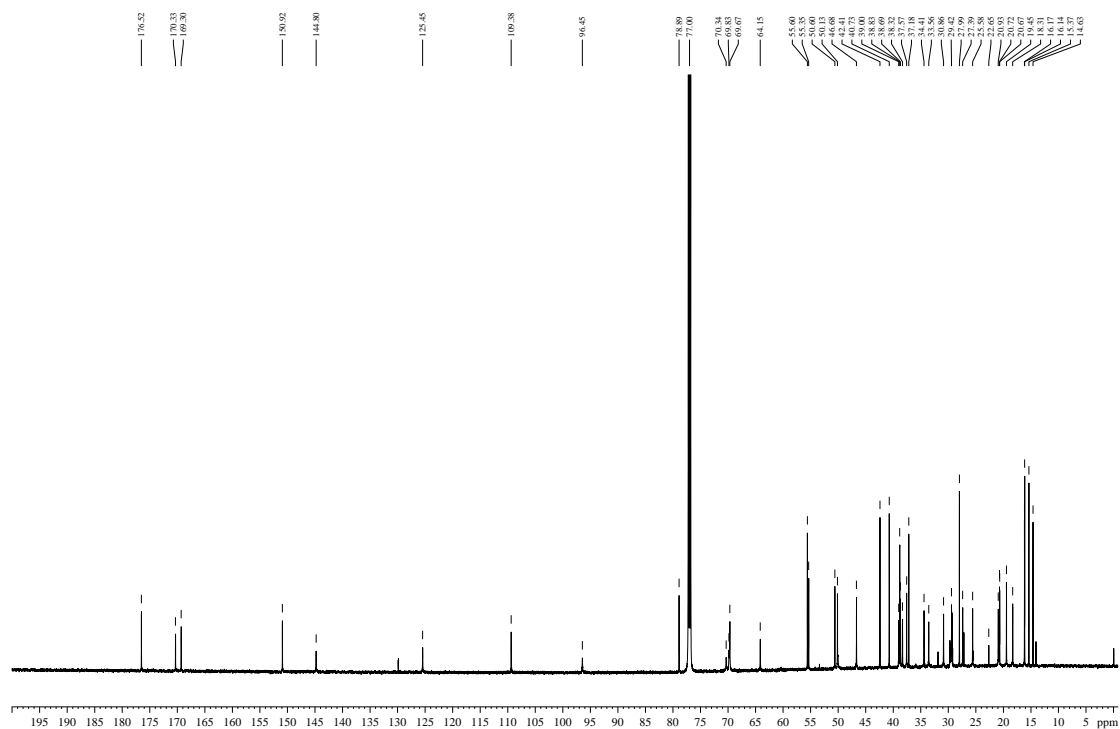
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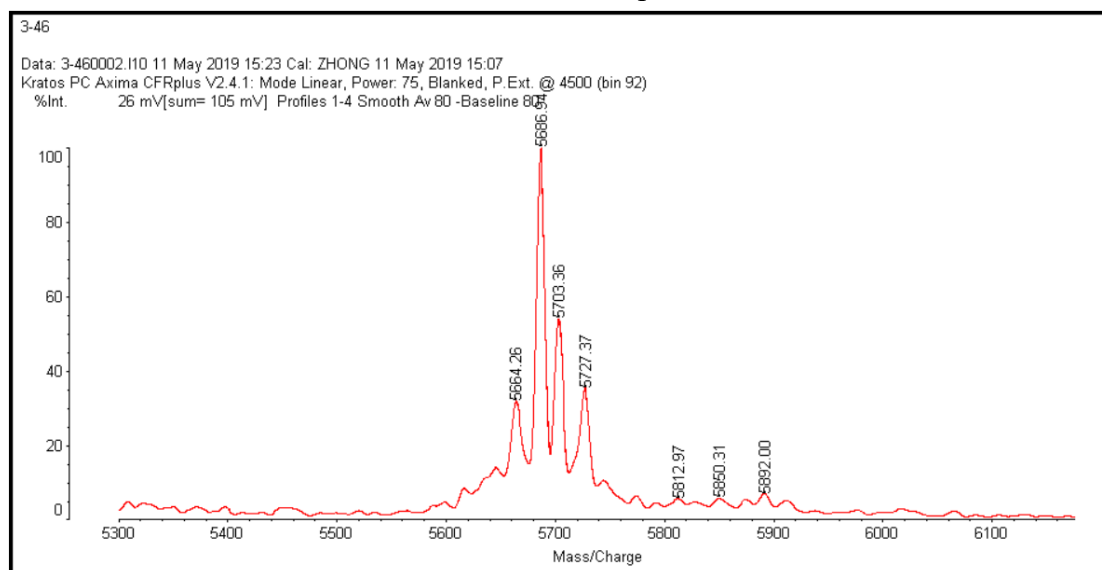
^1H NMR of compound **55**



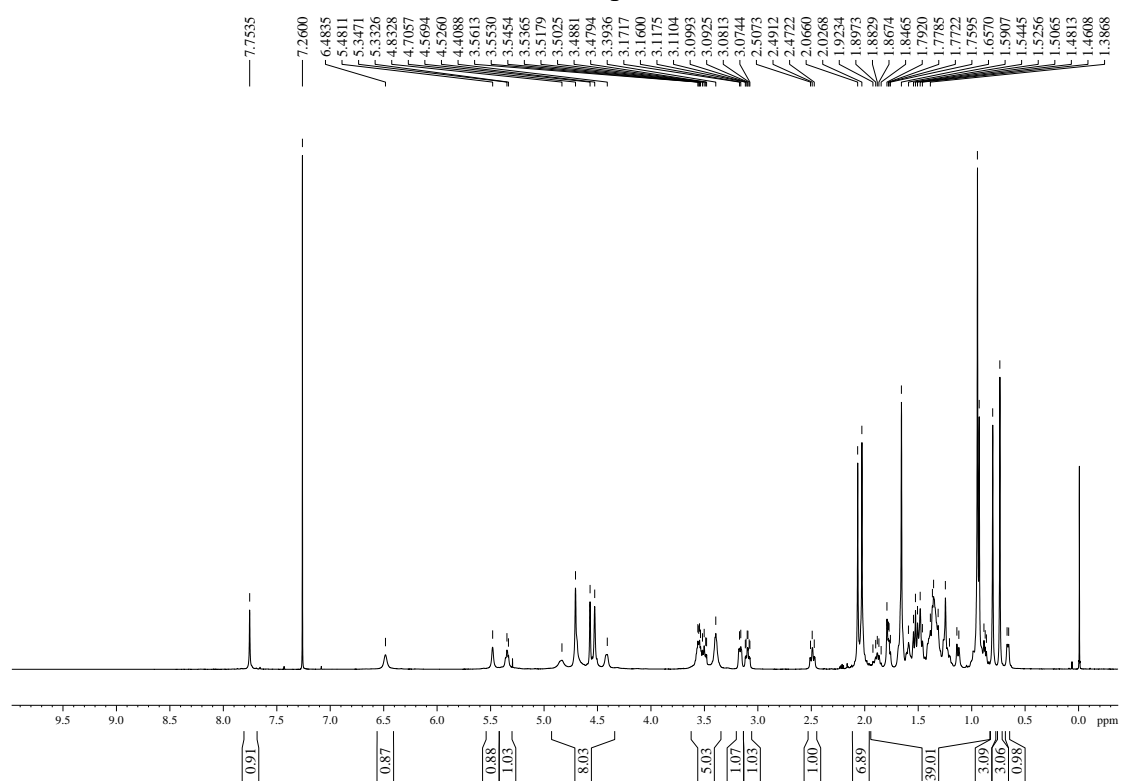
^{13}C NMR of compound **55**



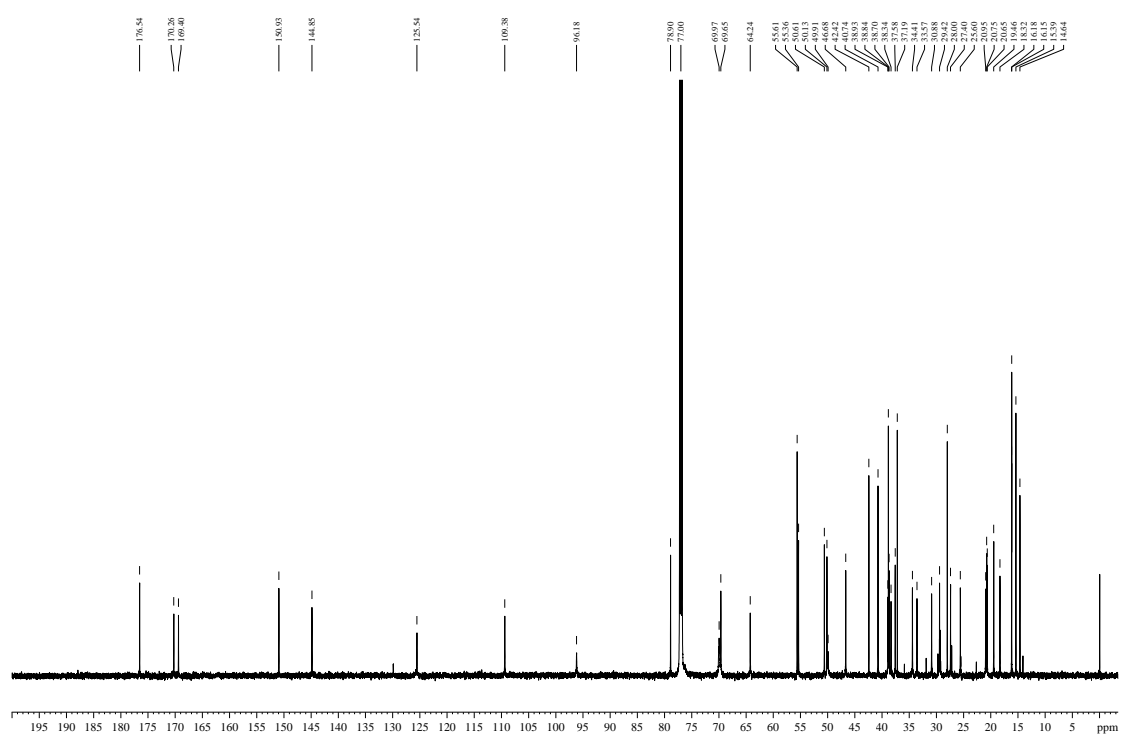
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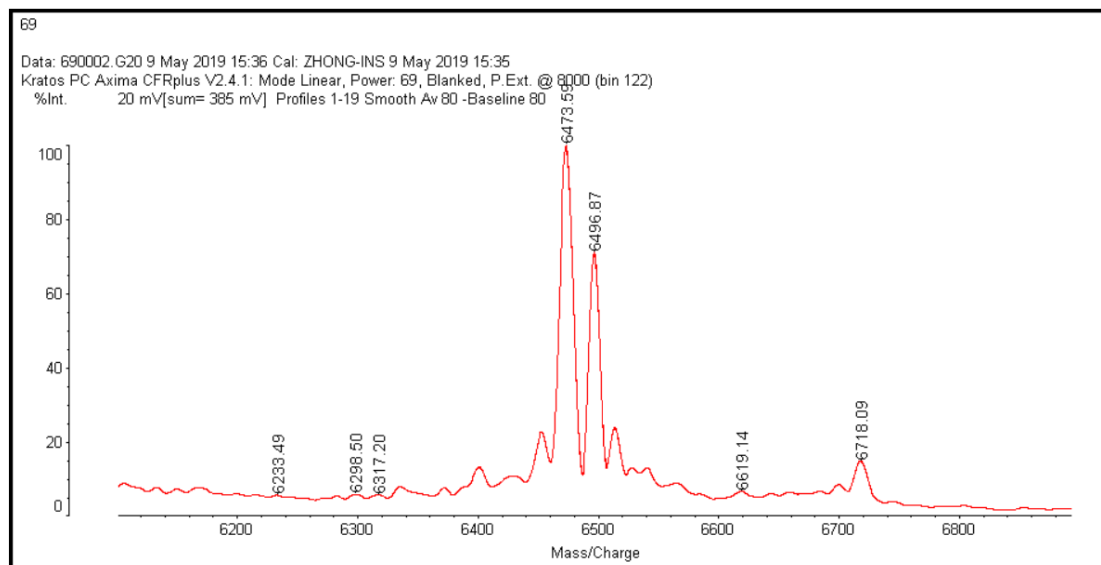
¹H NMR of compound **56**



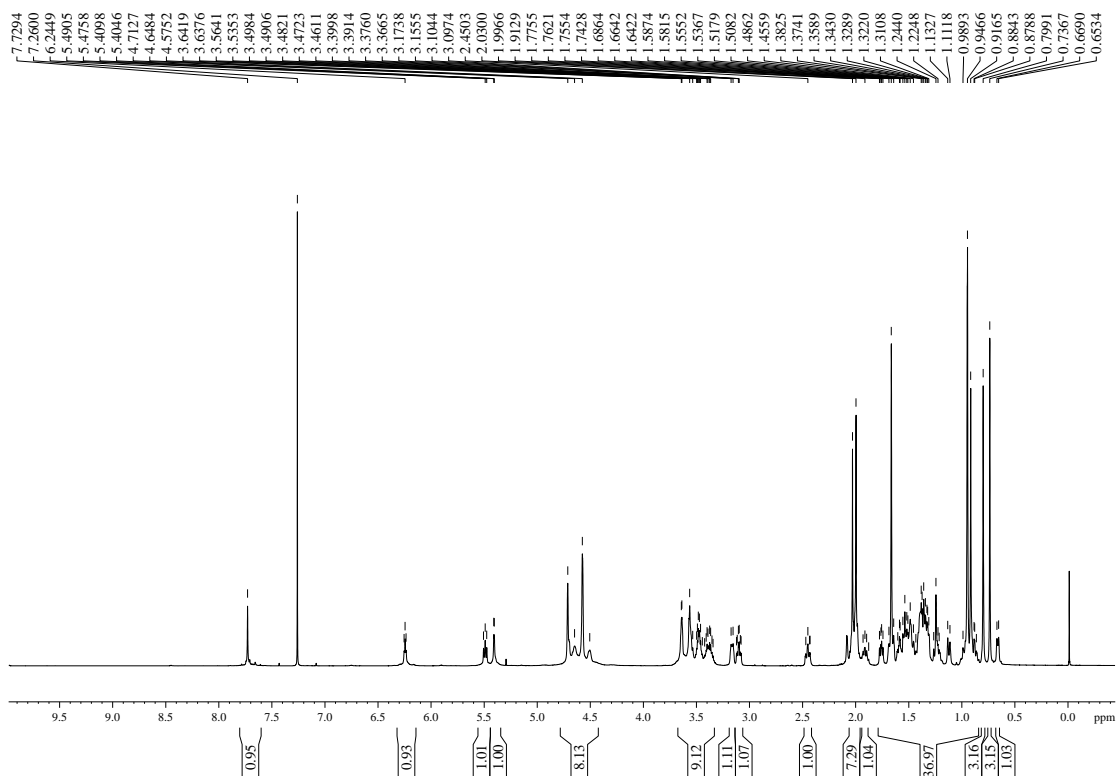
¹³C NMR of compound **56**



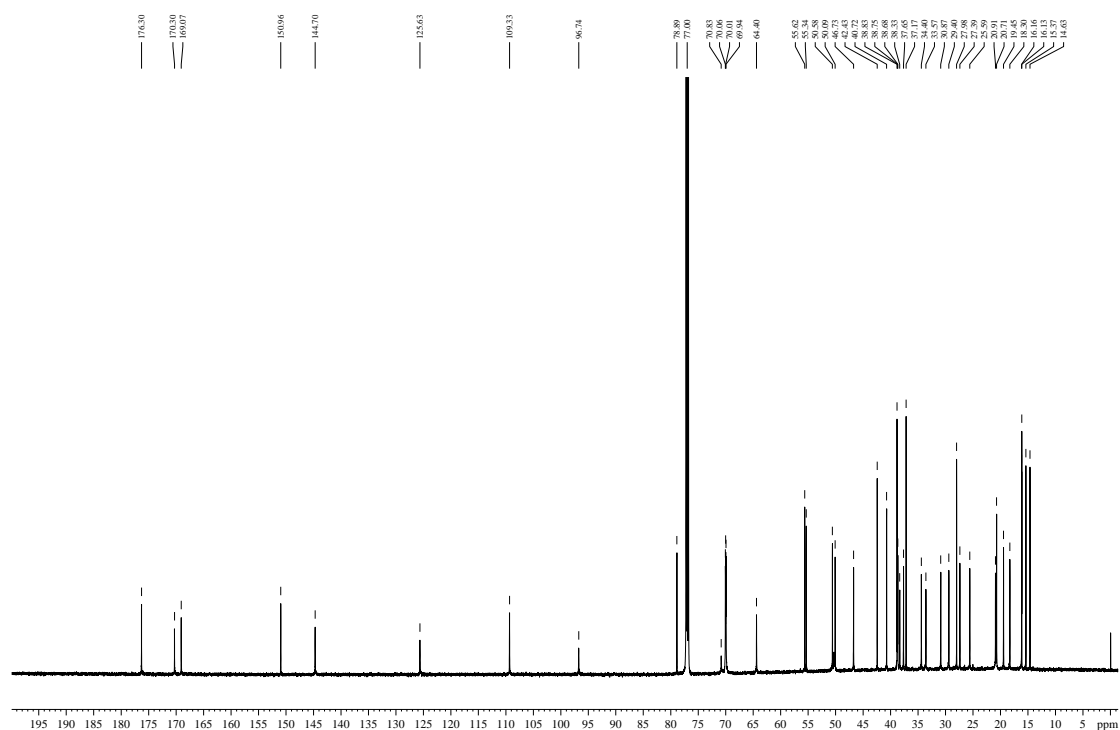
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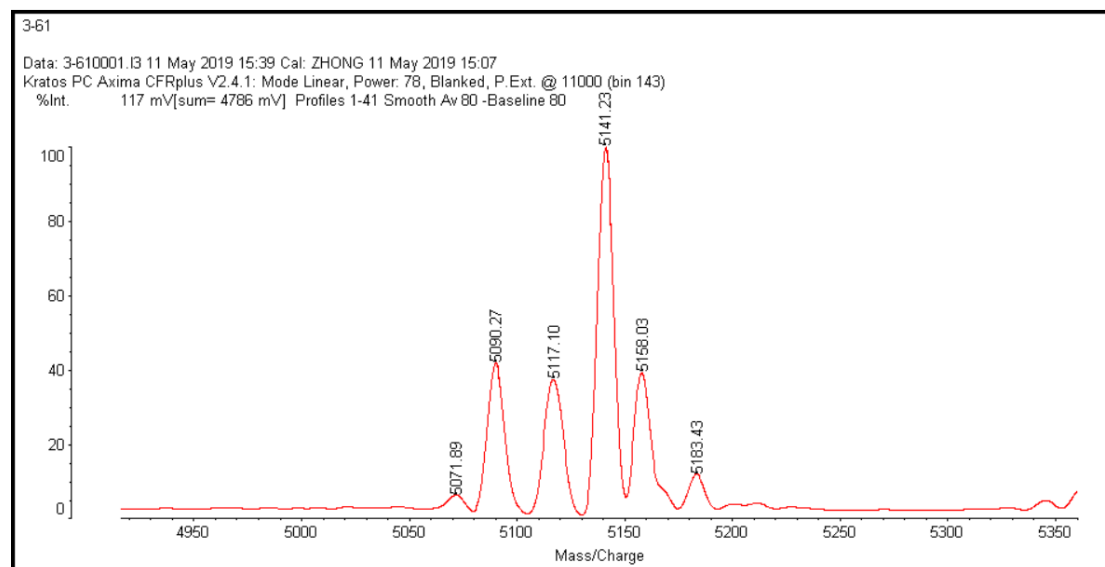
^1H NMR of compound **57**



¹³C NMR of compound **57**

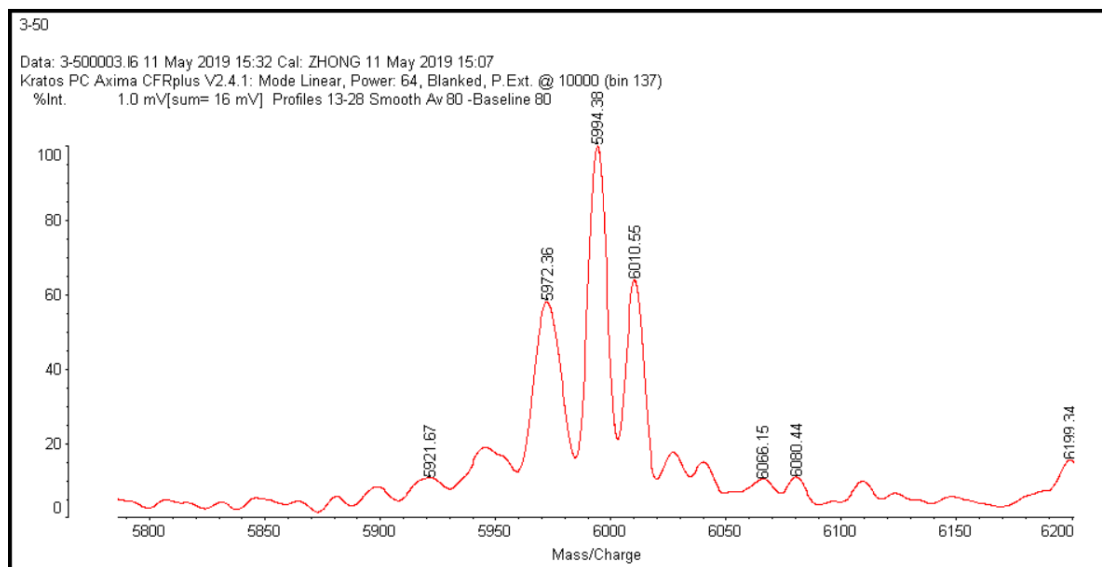


MALDI-TOF of compound **57**

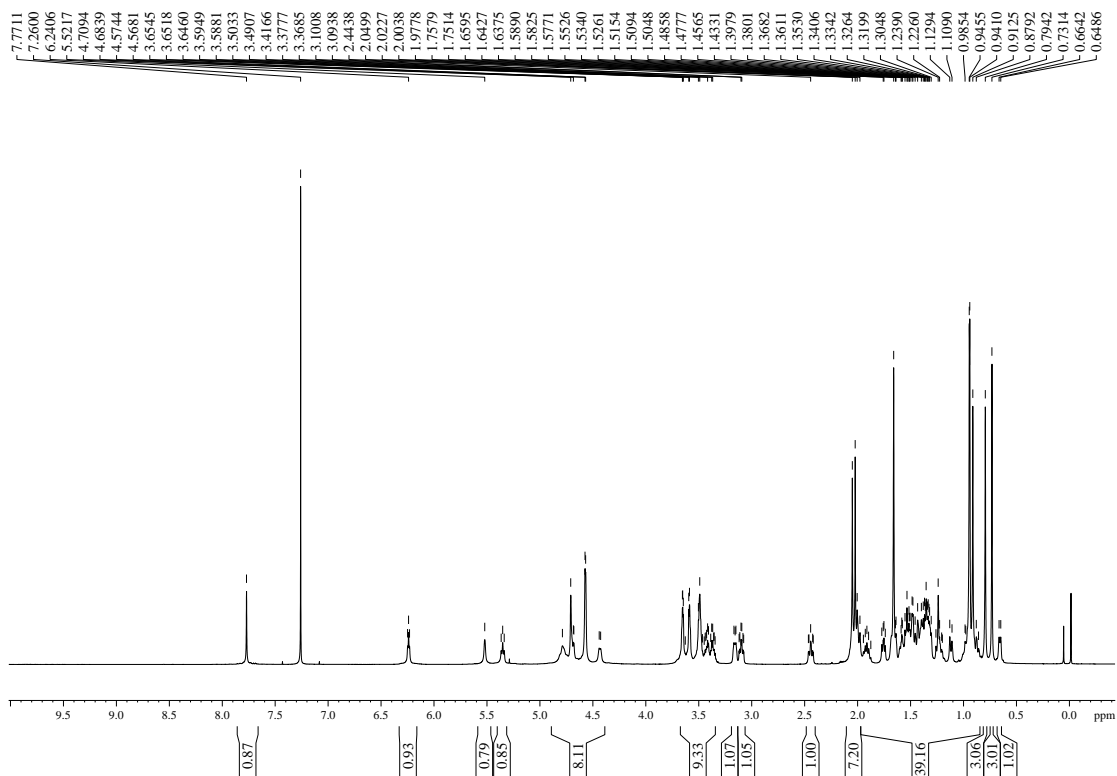


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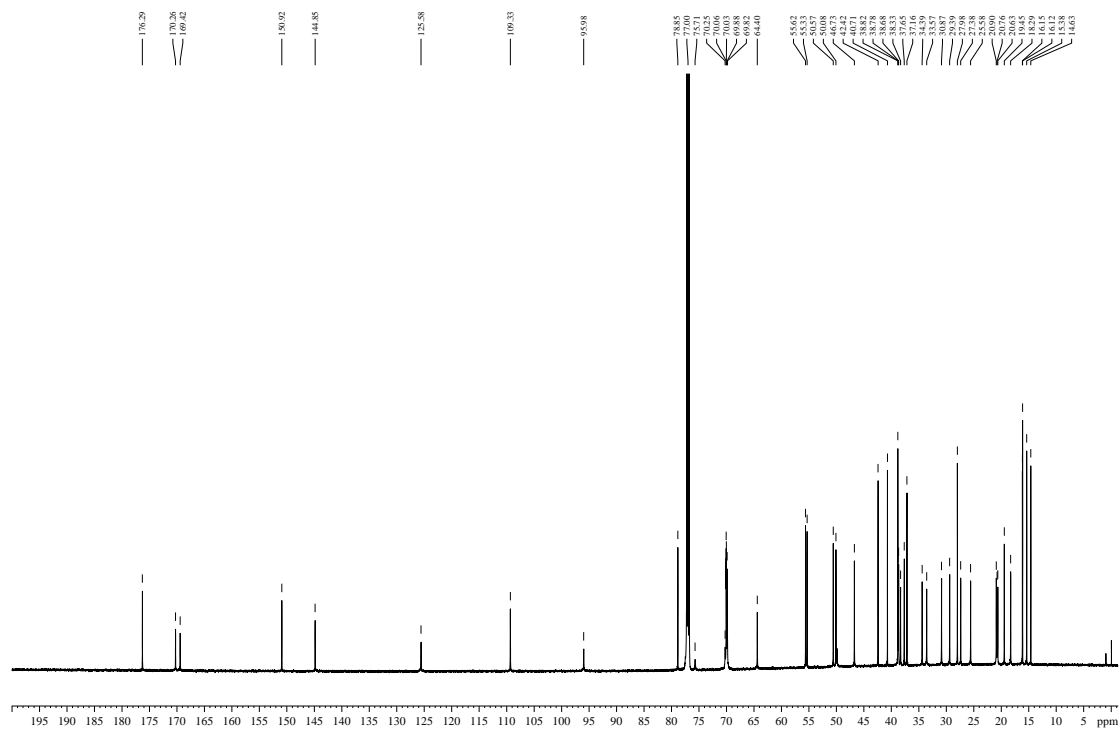
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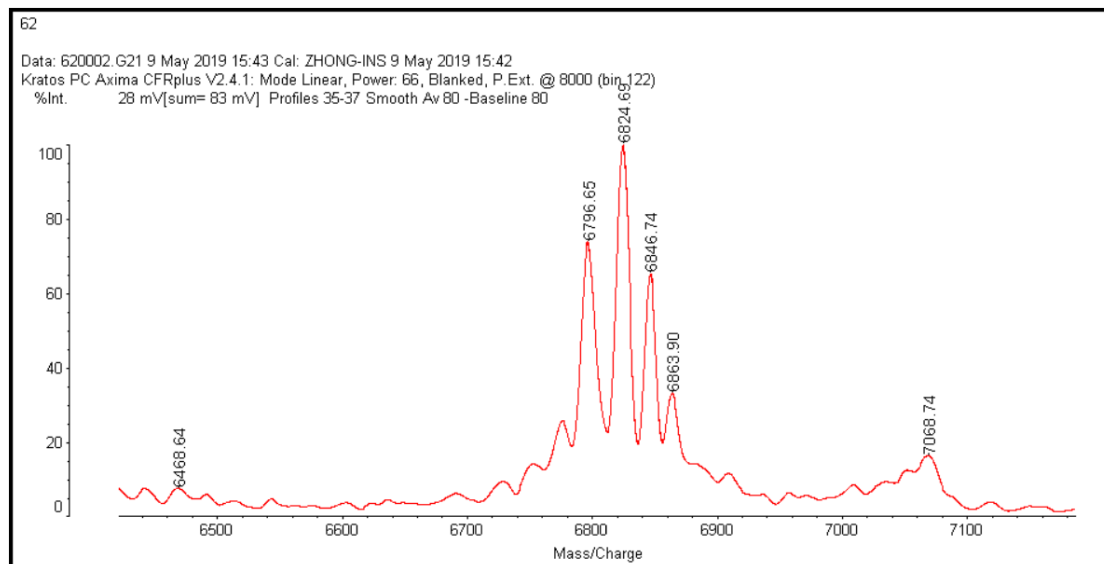
^1H NMR of compound **59**

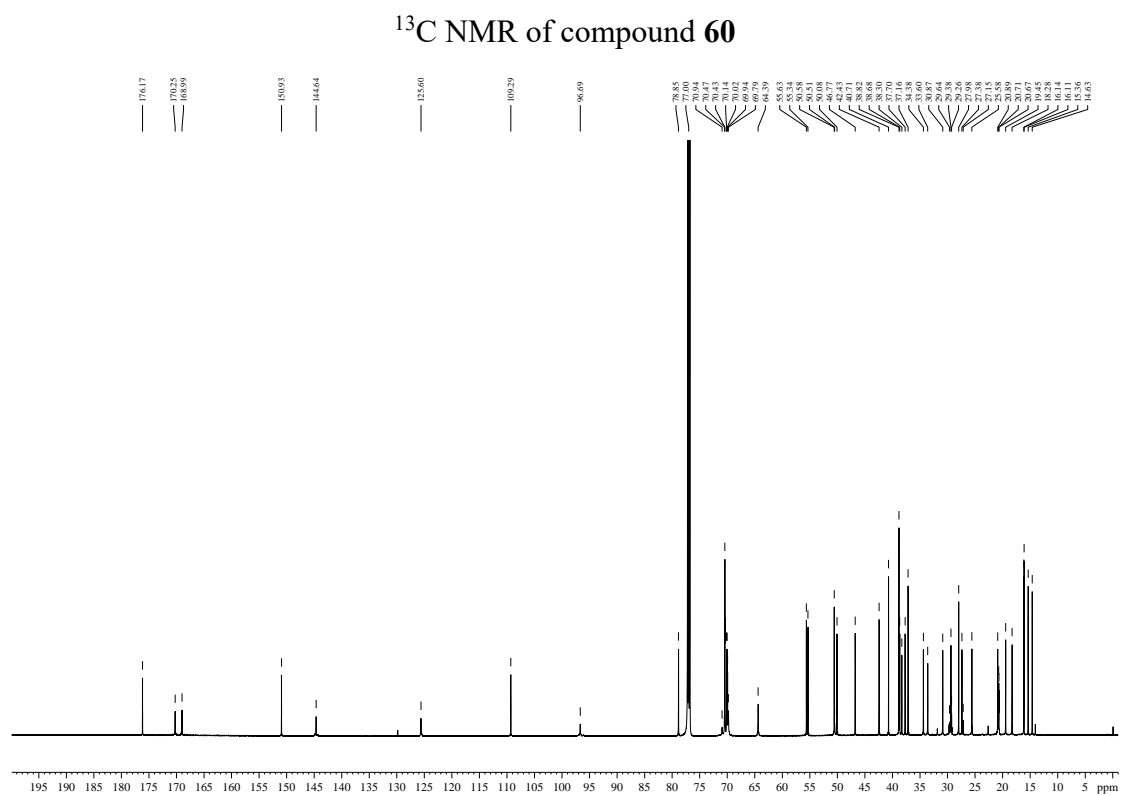
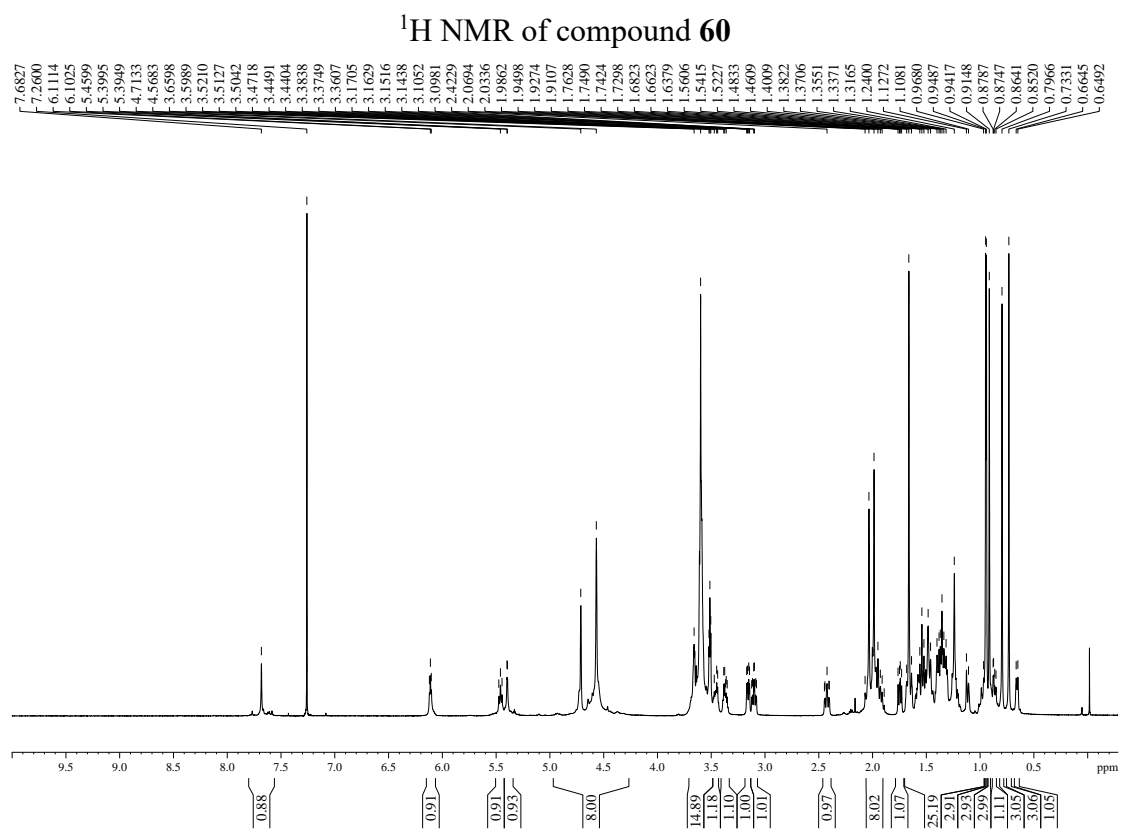


¹³C NMR of compound **59**

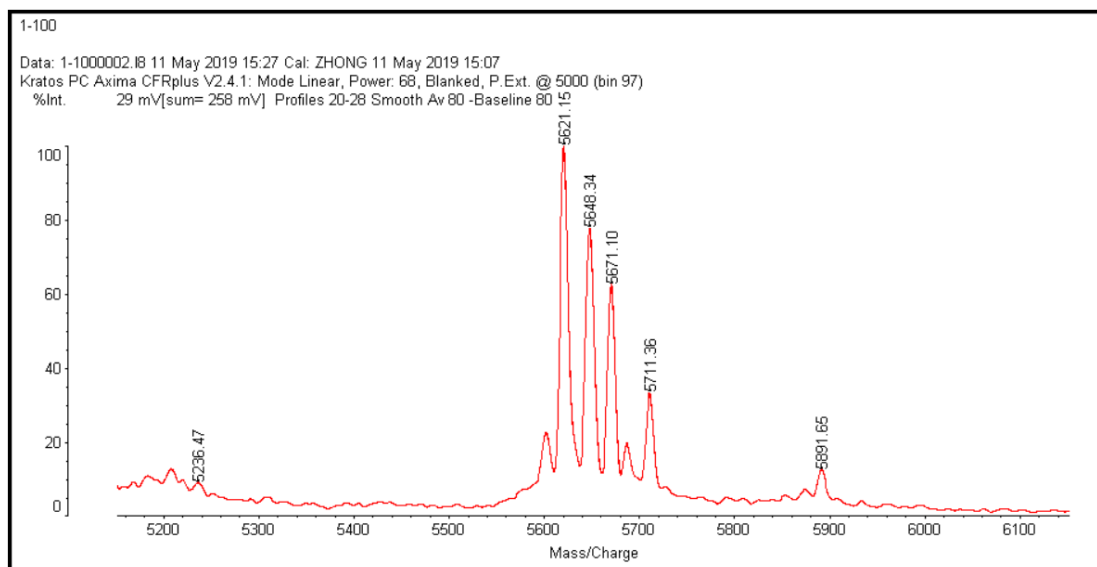


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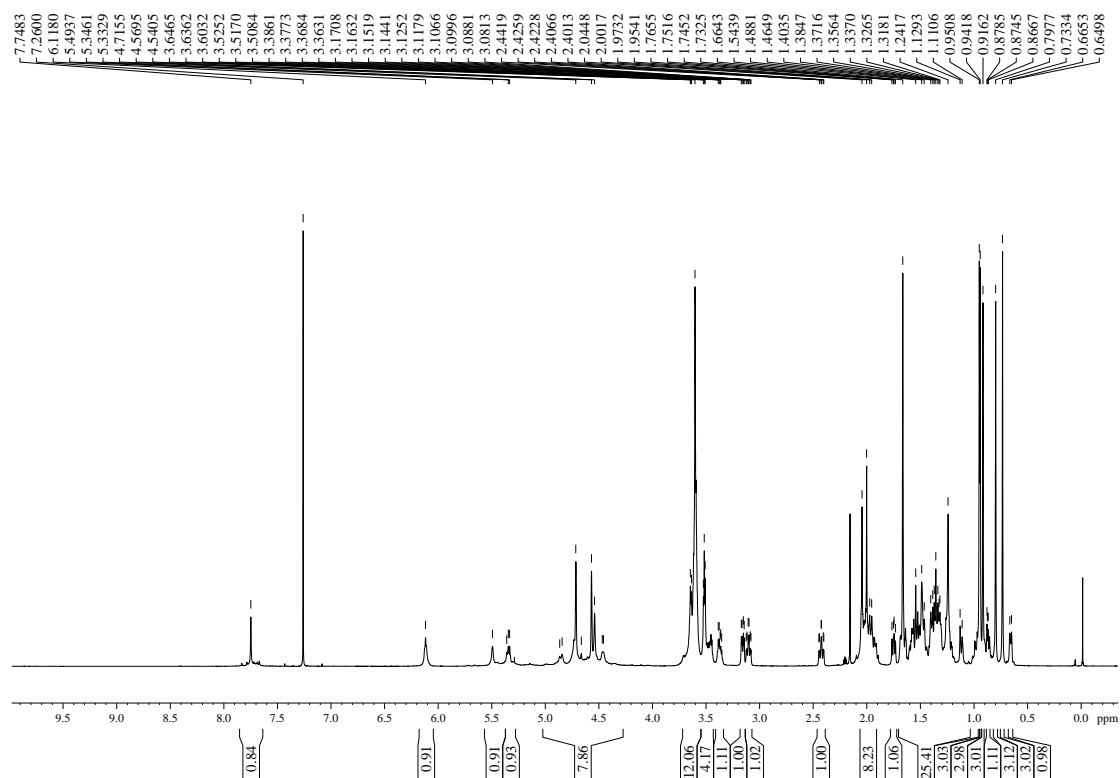




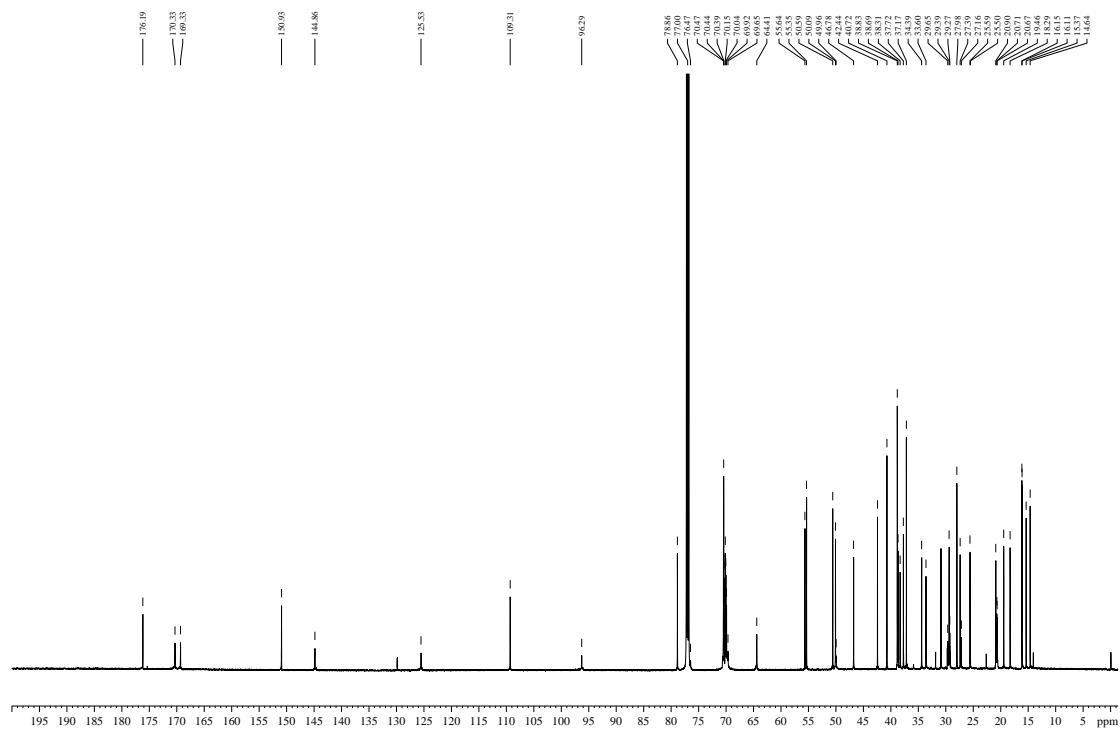
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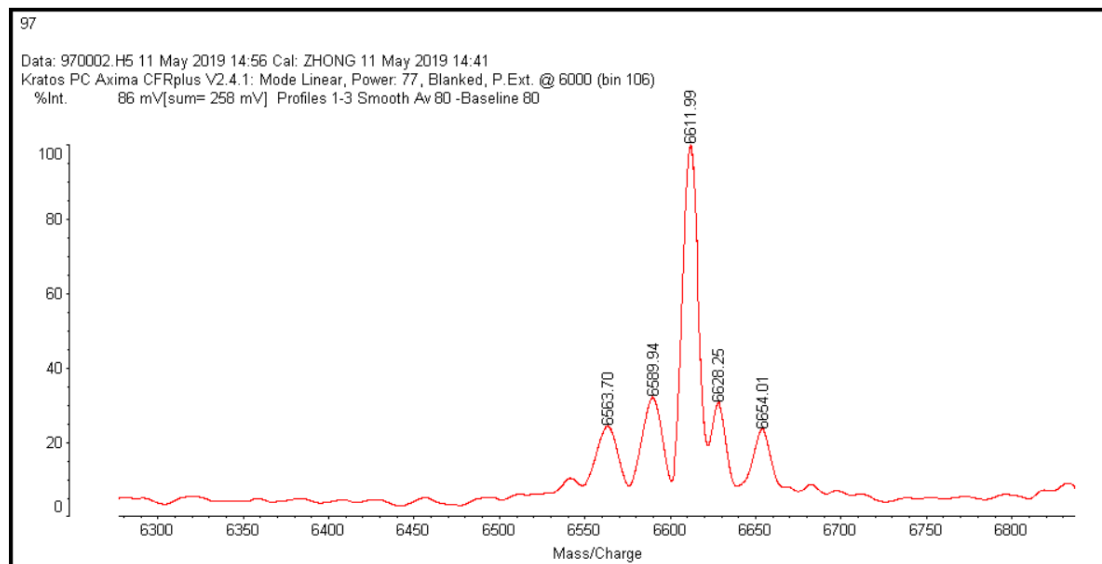
^1H NMR of compound **61**



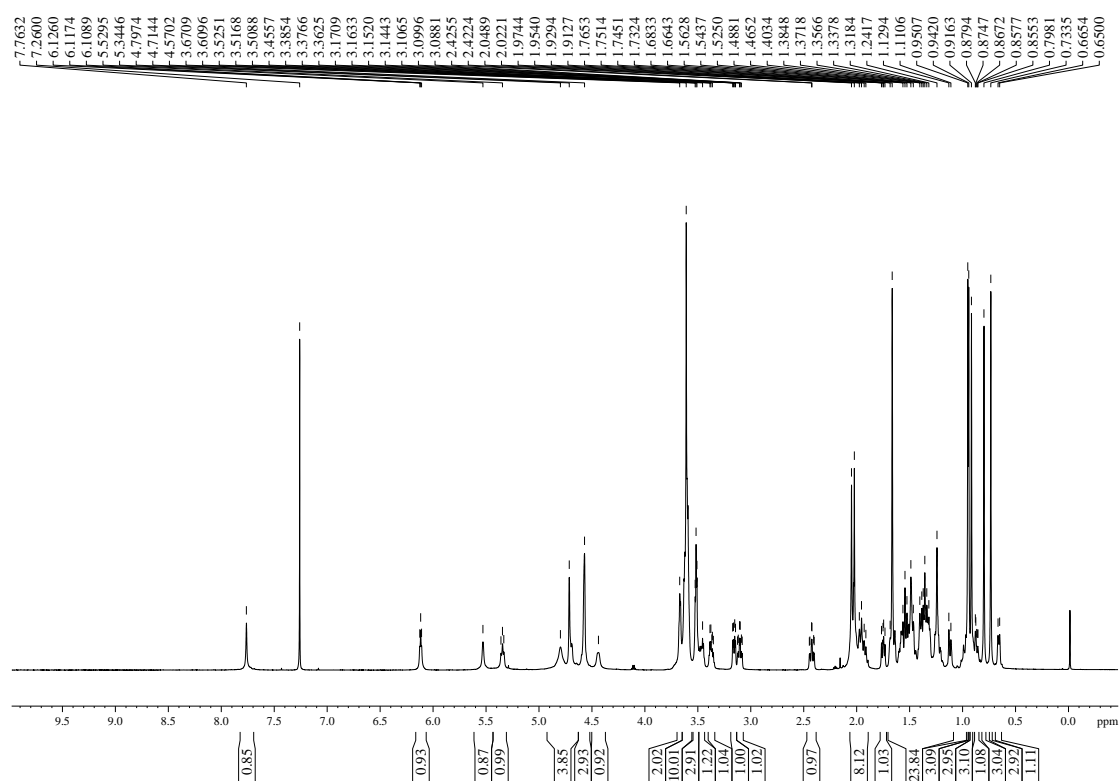
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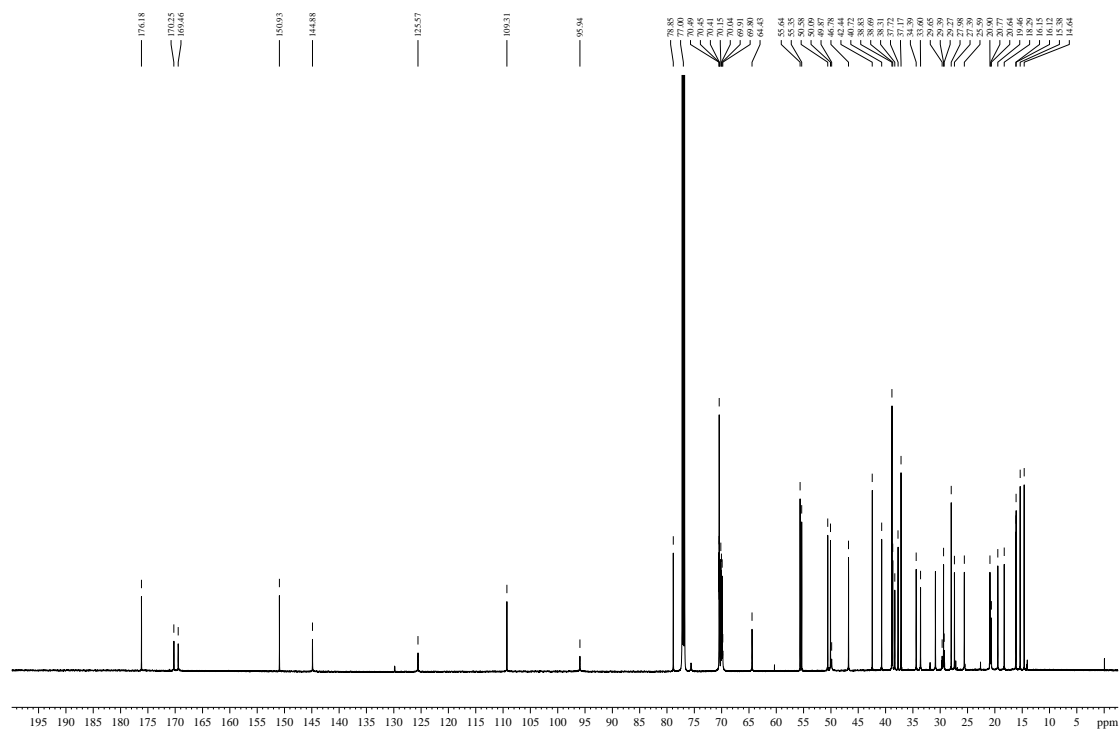
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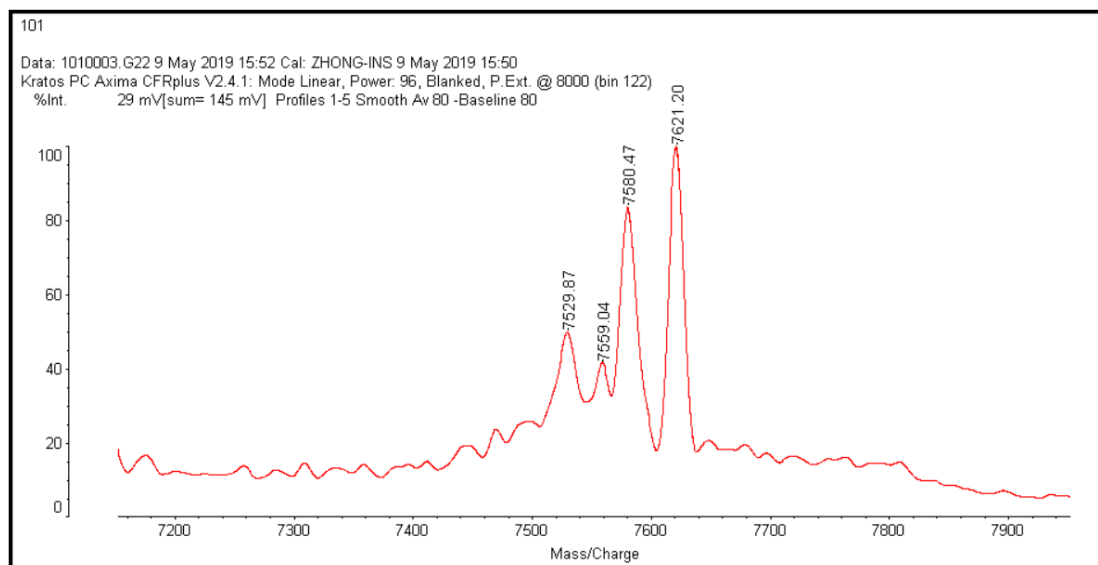
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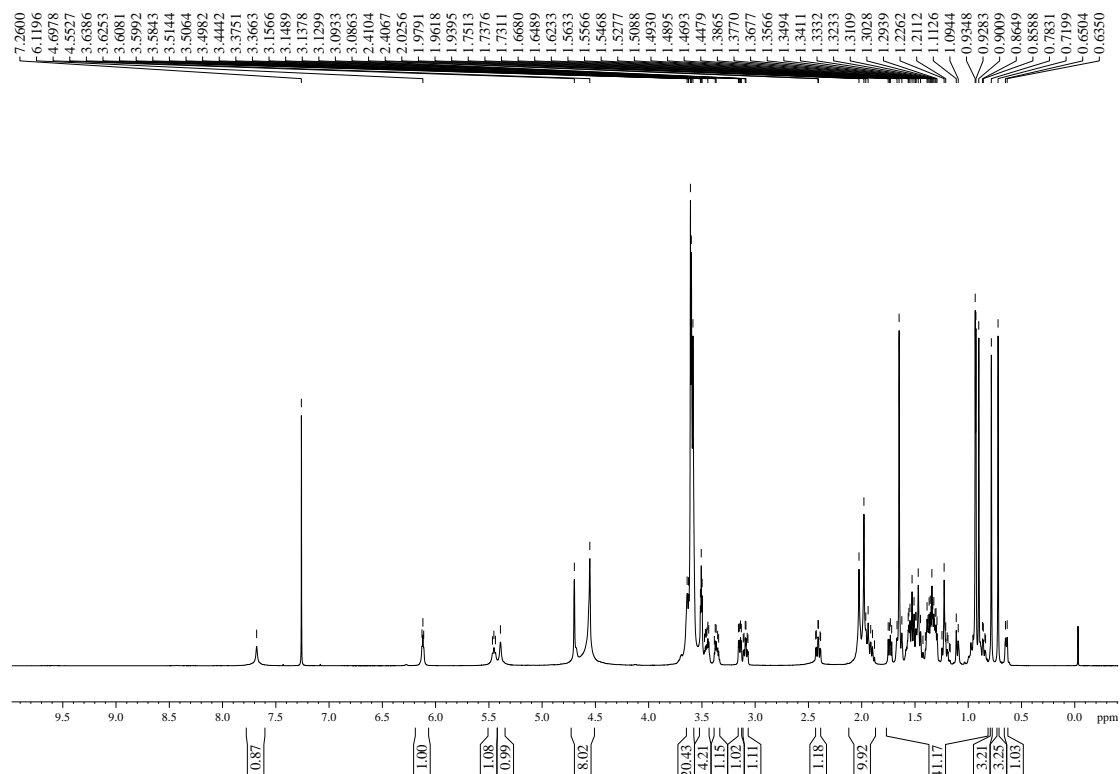
¹³C NMR of compound **62**



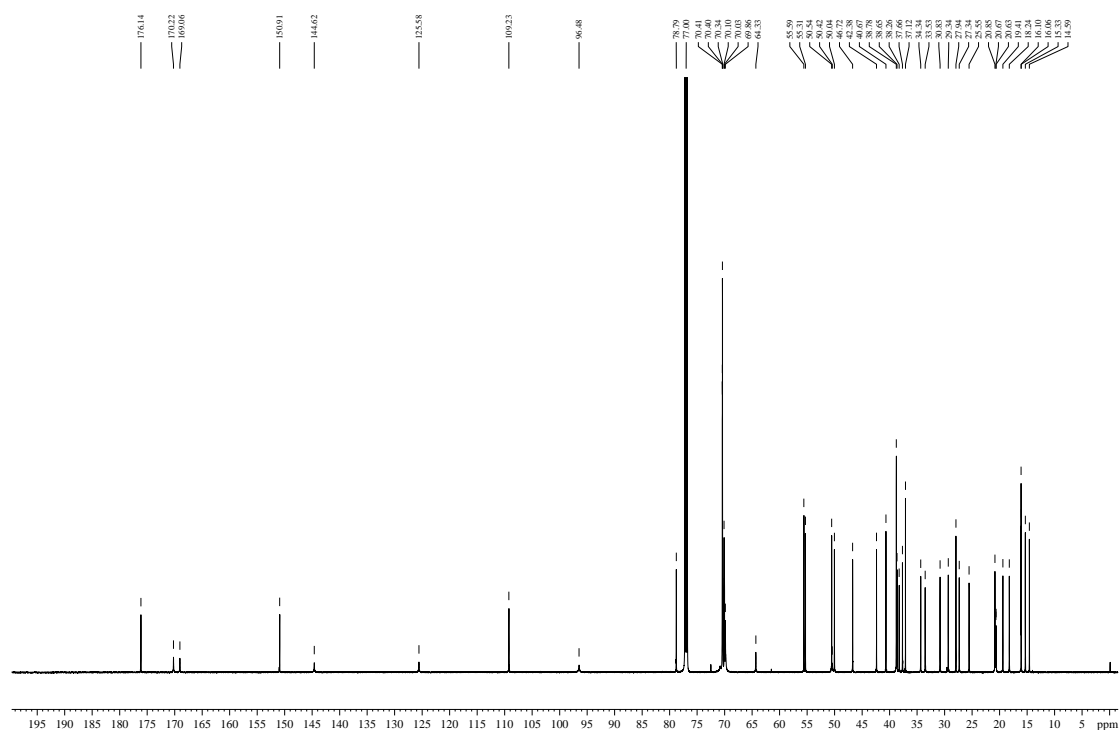
MALDI-TOF of compound **62**



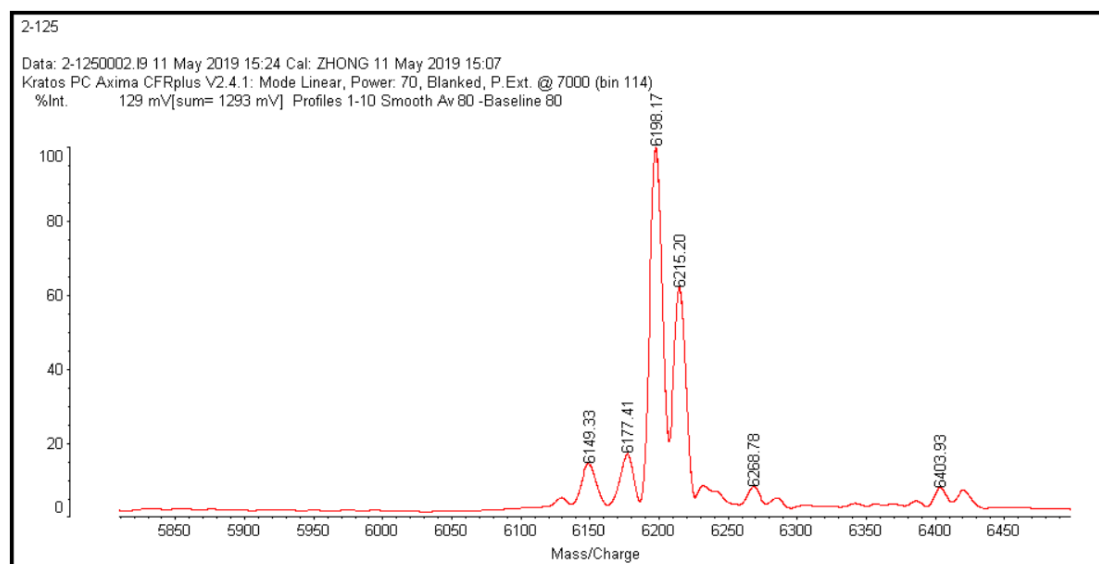
^1H NMR of compound **63**



^{13}C NMR of compound **63**



MALDI-TOF of compound **63**



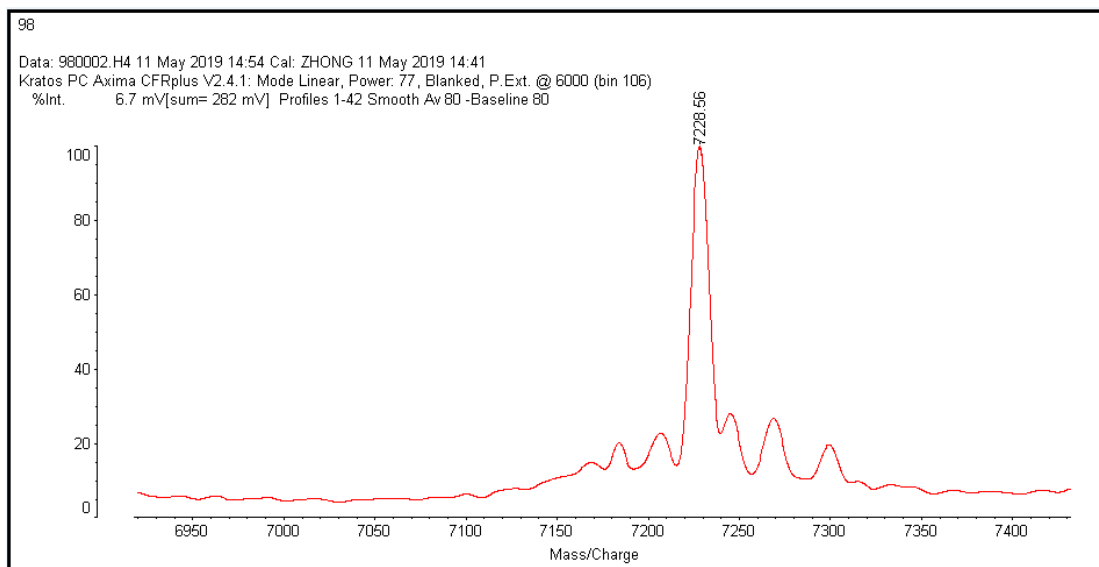
Chemical shifts (δ) listed on the right side of the spectrum (ppm): 7.7538, 7.2600, 6.1313, 4.7192, 4.5728, 4.5414, 3.6279, 3.6223, 3.6042, 3.5256, 3.5175, 3.4974, 3.4887, 3.4654, 3.4571, 3.3940, 3.3854, 3.1753, 3.1683, 3.1569, 3.1494, 3.1120, 3.1055, 2.4273, 2.0484, 2.0302, 2.0048, 1.9792, 1.9581, 1.9366, 1.9205, 1.7704, 1.7503, 1.7376, 1.6882, 1.6685, 1.6428, 1.5830, 1.5764, 1.5666, 1.5474, 1.5290, 1.5099, 1.4890, 1.4675, 1.4052, 1.3866, 1.3755, 1.3603, 1.3414, 1.3305, 1.3223, 1.3135, 1.2454, 1.1314, 1.1130, 0.9539, 0.9471, 0.9203, 0.8811, 0.8702, 0.8588, 0.8019, 0.7387, 0.6693, 0.6537.

17.230 17.034 16.955 14.657 12.539 10.330 9.630

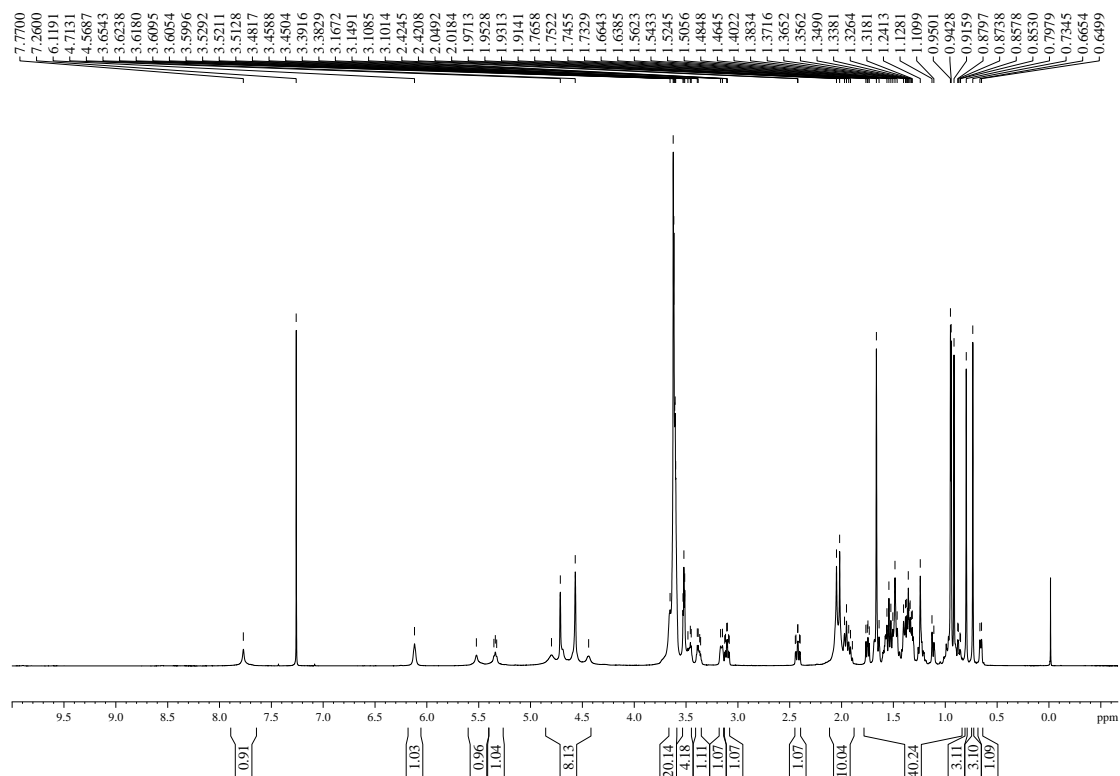
7.26 7.21 7.00 6.99 6.98 6.97 6.96 6.95 6.94 6.93 6.92 6.91 6.90 6.89 6.88 6.87 6.86 6.85 6.84 6.83 6.82 6.81 6.80 6.79 6.78 6.77 6.76 6.75 6.74 6.73 6.72 6.71 6.70 6.69 6.68 6.67 6.66 6.65 6.64 6.63 6.62 6.61 6.60 6.59 6.58 6.57 6.56 6.55 6.54 6.53 6.52 6.51 6.50 6.49 6.48 6.47 6.46 6.45 6.44 6.43 6.42 6.41 6.40 6.39 6.38 6.37 6.36 6.35 6.34 6.33 6.32 6.31 6.30 6.29 6.28 6.27 6.26 6.25 6.24 6.23 6.22 6.21 6.20 6.19 6.18 6.17 6.16 6.15 6.14 6.13 6.12 6.11 6.10 6.09 6.08 6.07 6.06 6.05 6.04 6.03 6.02 6.01 6.00 5.99 5.98 5.97 5.96 5.95 5.94 5.93 5.92 5.91 5.90 5.89 5.88 5.87 5.86 5.85 5.84 5.83 5.82 5.81 5.80 5.79 5.78 5.77 5.76 5.75 5.74 5.73 5.72 5.71 5.70 5.69 5.68 5.67 5.66 5.65 5.64 5.63 5.62 5.61 5.60 5.59 5.58 5.57 5.56 5.55 5.54 5.53 5.52 5.51 5.50 5.49 5.48 5.47 5.46 5.45 5.44 5.43 5.42 5.41 5.40 5.39 5.38 5.37 5.36 5.35 5.34 5.33 5.32 5.31 5.30 5.29 5.28 5.27 5.26 5.25 5.24 5.23 5.22 5.21 5.20 5.19 5.18 5.17 5.16 5.15 5.14 5.13 5.12 5.11 5.10 5.09 5.08 5.07 5.06 5.05 5.04 5.03 5.02 5.01 5.00 4.99 4.98 4.97 4.96 4.95 4.94 4.93 4.92 4.91 4.90 4.89 4.88 4.87 4.86 4.85 4.84 4.83 4.82 4.81 4.80 4.79 4.78 4.77 4.76 4.75 4.74 4.73 4.72 4.71 4.70 4.69 4.68 4.67 4.66 4.65 4.64 4.63 4.62 4.61 4.60 4.59 4.58 4.57 4.56 4.55 4.54 4.53 4.52 4.51 4.50 4.49 4.48 4.47 4.46 4.45 4.44 4.43 4.42 4.41 4.40 4.39 4.38 4.37 4.36 4.35 4.34 4.33 4.32 4.31 4.30 4.29 4.28 4.27 4.26 4.25 4.24 4.23 4.22 4.21 4.20 4.19 4.18 4.17 4.16 4.15 4.14 4.13 4.12 4.11 4.10 4.09 4.08 4.07 4.06 4.05 4.04 4.03 4.02 4.01 4.00 3.99 3.98 3.97 3.96 3.95 3.94 3.93 3.92 3.91 3.90 3.89 3.88 3.87 3.86 3.85 3.84 3.83 3.82 3.81 3.80 3.79 3.78 3.77 3.76 3.75 3.74 3.73 3.72 3.71 3.70 3.69 3.68 3.67 3.66 3.65 3.64 3.63 3.62 3.61 3.60 3.59 3.58 3.57 3.56 3.55 3.54 3.53 3.52 3.51 3.50 3.49 3.48 3.47 3.46 3.45 3.44 3.43 3.42 3.41 3.40 3.39 3.38 3.37 3.36 3.35 3.34 3.33 3.32 3.31 3.30 3.29 3.28 3.27 3.26 3.25 3.24 3.23 3.22 3.21 3.20 3.19 3.18 3.17 3.16 3.15 3.14 3.13 3.12 3.11 3.10 3.09 3.08 3.07 3.06 3.05 3.04 3.03 3.02 3.01 3.00 2.99 2.98 2.97 2.96 2.95 2.94 2.93 2.92 2.91 2.90 2.89 2.88 2.87 2.86 2.85 2.84 2.83 2.82 2.81 2.80 2.79 2.78 2.77 2.76 2.75 2.74 2.73 2.72 2.71 2.70 2.69 2.68 2.67 2.66 2.65 2.64 2.63 2.62 2.61 2.60 2.59 2.58 2.57 2.56 2.55 2.54 2.53 2.52 2.51 2.50 2.49 2.48 2.47 2.46 2.45 2.44 2.43 2.42 2.41 2.40 2.39 2.38 2.37 2.36 2.35 2.34 2.33 2.32 2.31 2.30 2.29 2.28 2.27 2.26 2.25 2.24 2.23 2.22 2.21 2.20 2.19 2.18 2.17 2.16 2.15 2.14 2.13 2.12 2.11 2.10 2.09 2.08 2.07 2.06 2.05 2.04 2.03 2.02 2.01 2.00 1.99 1.98 1.97 1.96 1.95 1.94 1.93 1.92 1.91 1.90 1.89 1.88 1.87 1.86 1.85 1.84 1.83 1.82 1.81 1.80 1.79 1.78 1.77 1.76 1.75 1.74 1.73 1.72 1.71 1.70 1.69 1.68 1.67 1.66 1.65 1.64 1.63 1.62 1.61 1.60 1.59 1.58 1.57 1.56 1.55 1.54 1.53 1.52 1.51 1.50 1.49 1.48 1.47 1.46 1.45 1.44 1.43 1.42 1.41 1.40 1.39 1.38 1.37 1.36 1.35 1.34 1.33 1.32 1.31 1.30 1.29 1.28 1.27 1.26 1.25 1.24 1.23 1.22 1.21 1.20 1.19 1.18 1.17 1.16 1.15 1.14 1.13 1.12 1.11 1.10 1.09 1.08 1.07 1.06 1.05 1.04 1.03 1.02 1.01 1.00 0.99 0.98 0.97 0.96 0.95 0.94 0.93 0.92 0.91 0.90 0.89 0.88 0.87 0.86 0.85 0.84 0.83 0.82 0.81 0.80 0.79 0.78 0.77 0.76 0.75 0.74 0.73 0.72 0.71 0.70 0.69 0.68 0.67 0.66 0.65 0.64 0.63 0.62 0.61 0.60 0.59 0.58 0.57 0.56 0.55 0.54 0.53 0.52 0.51 0.50 0.49 0.48 0.47 0.46 0.45 0.44 0.43 0.42 0.41 0.40 0.39 0.38 0.37 0.36 0.35 0.34 0.33 0.32 0.31 0.30 0.29 0.28 0.27 0.26 0.25 0.24 0.23 0.22 0.21 0.20 0.19 0.18 0.17 0.16 0.15 0.14 0.13 0.12 0.11 0.10 0.09 0.08 0.07 0.06 0.05 0.04 0.03 0.02 0.01 0.00

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Date_ 20181013
Time 10.30
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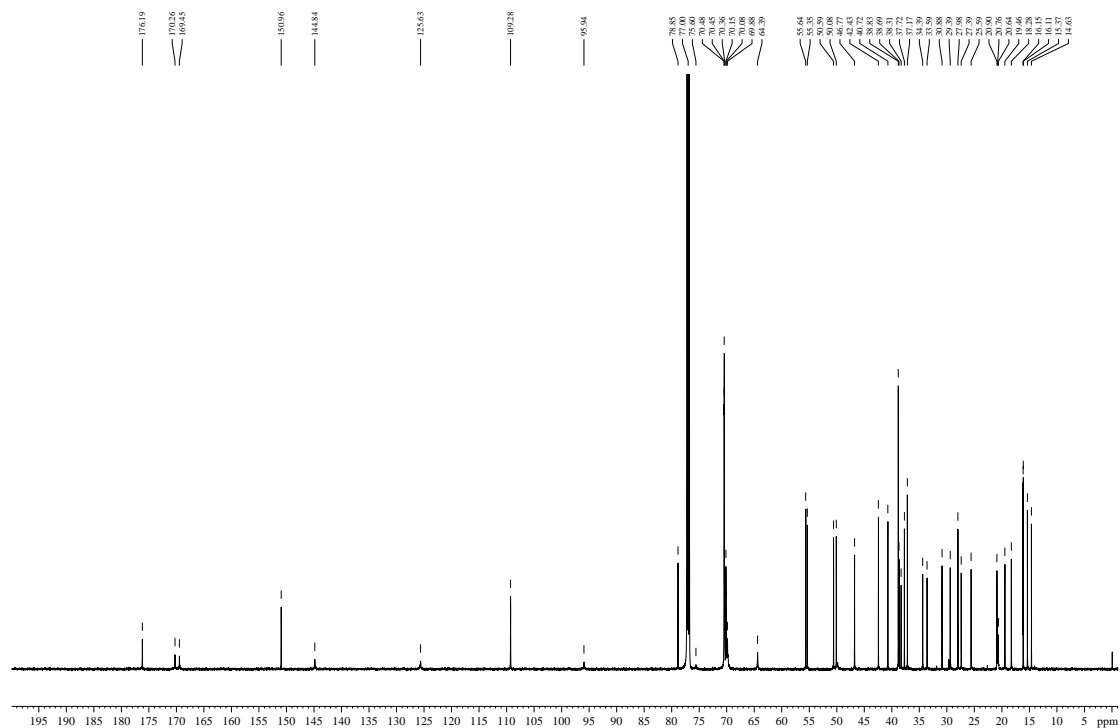
MALDI-TOF of compound **64**



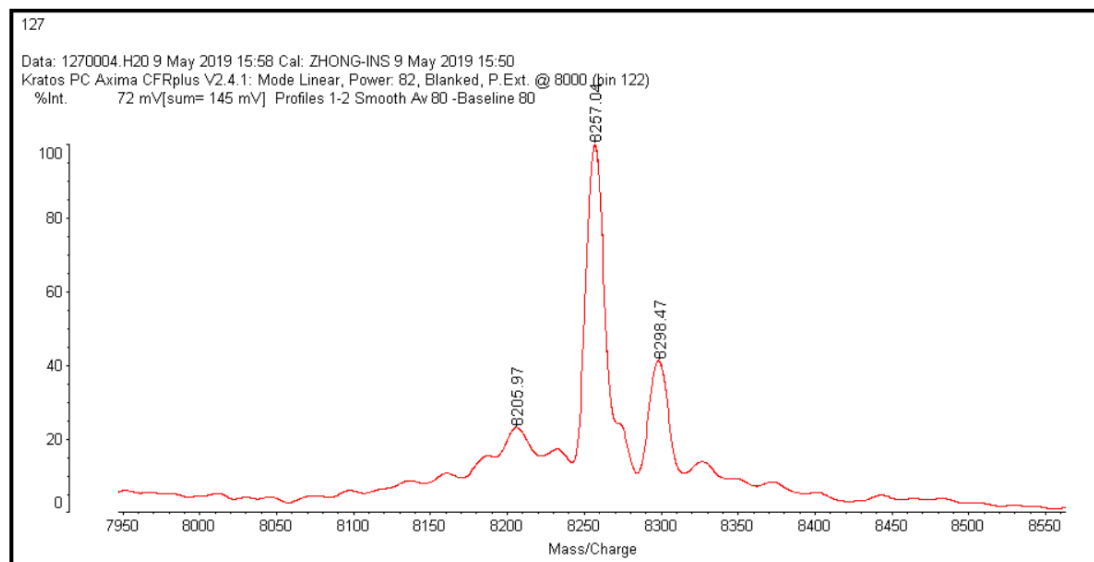
^1H NMR of compound **65**



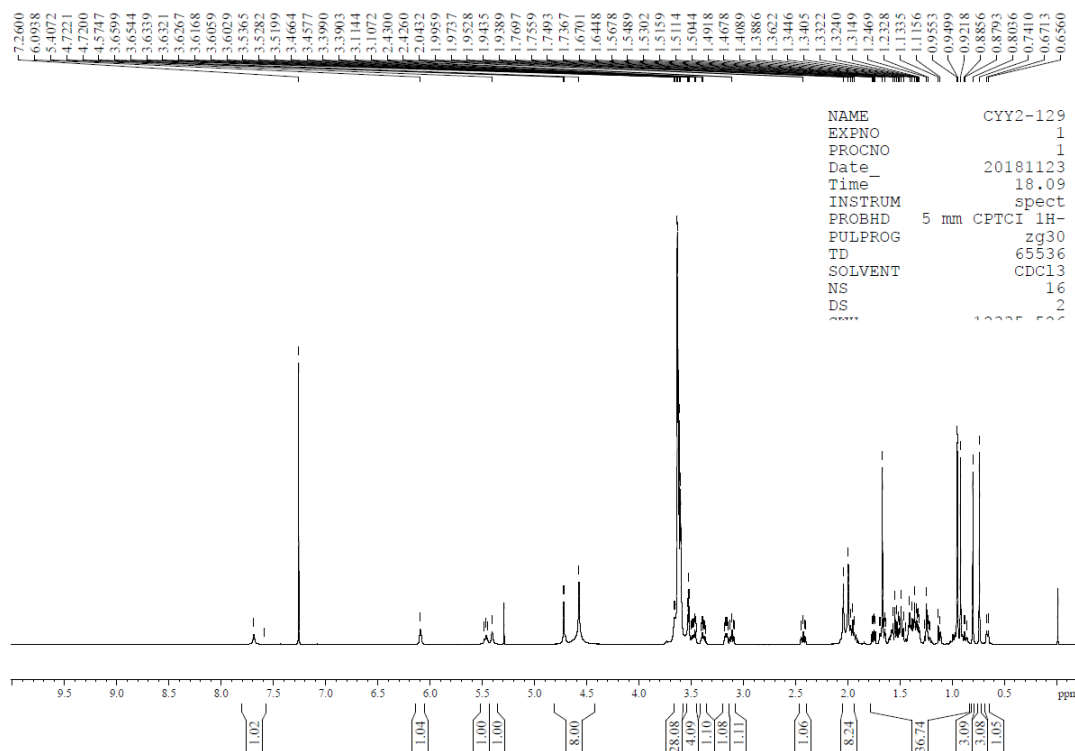
¹³C NMR of compound **65**



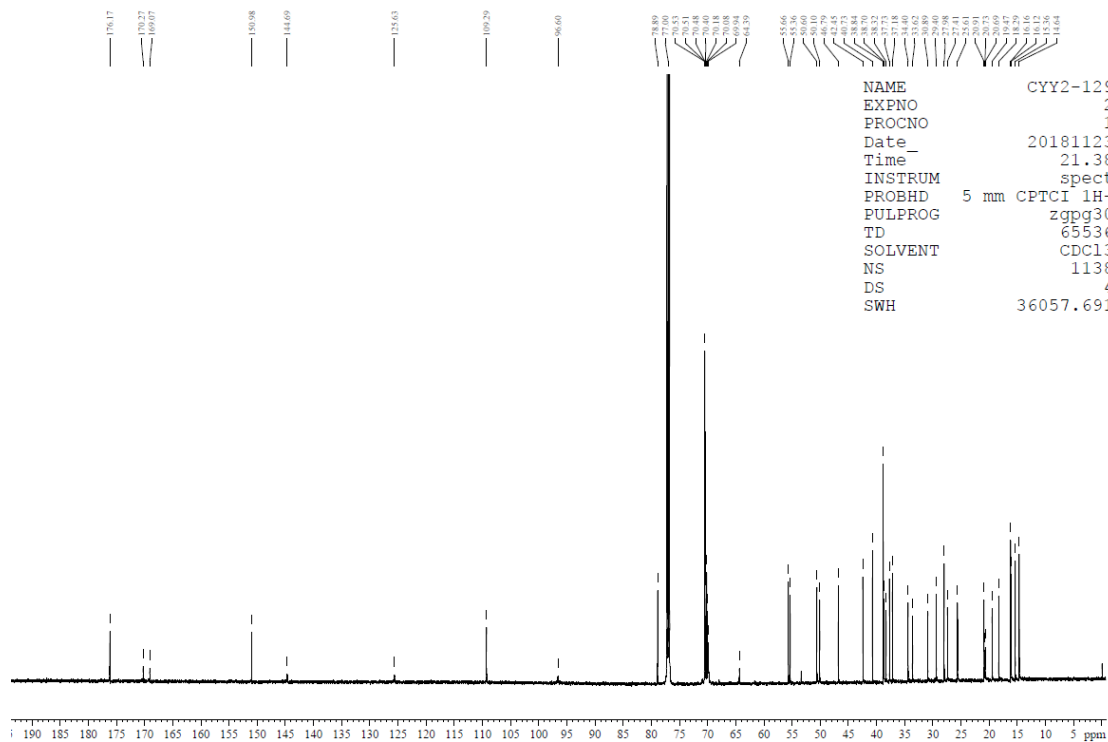
MALDI-TOF of compound **65**



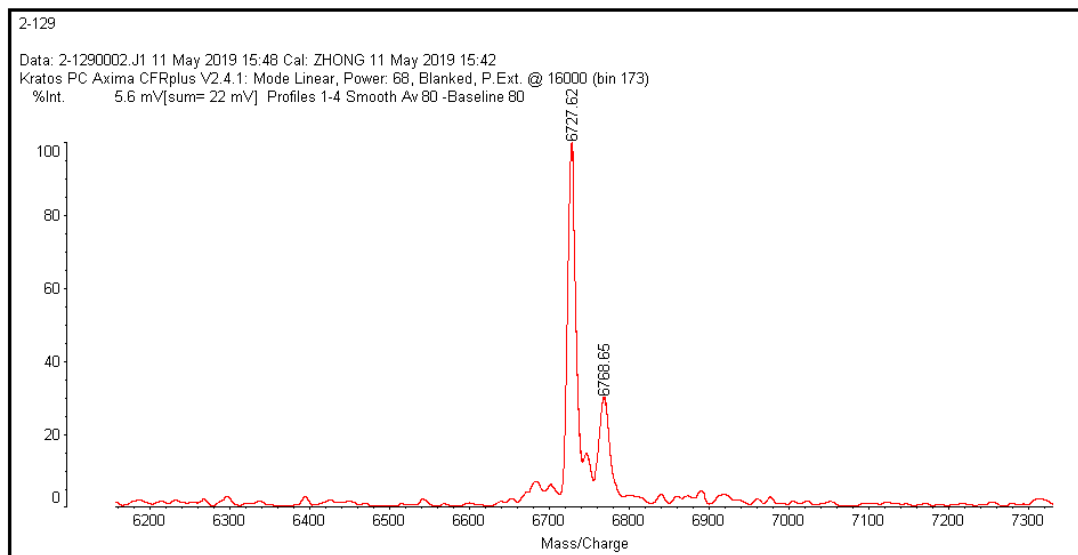
¹H NMR of compound 66



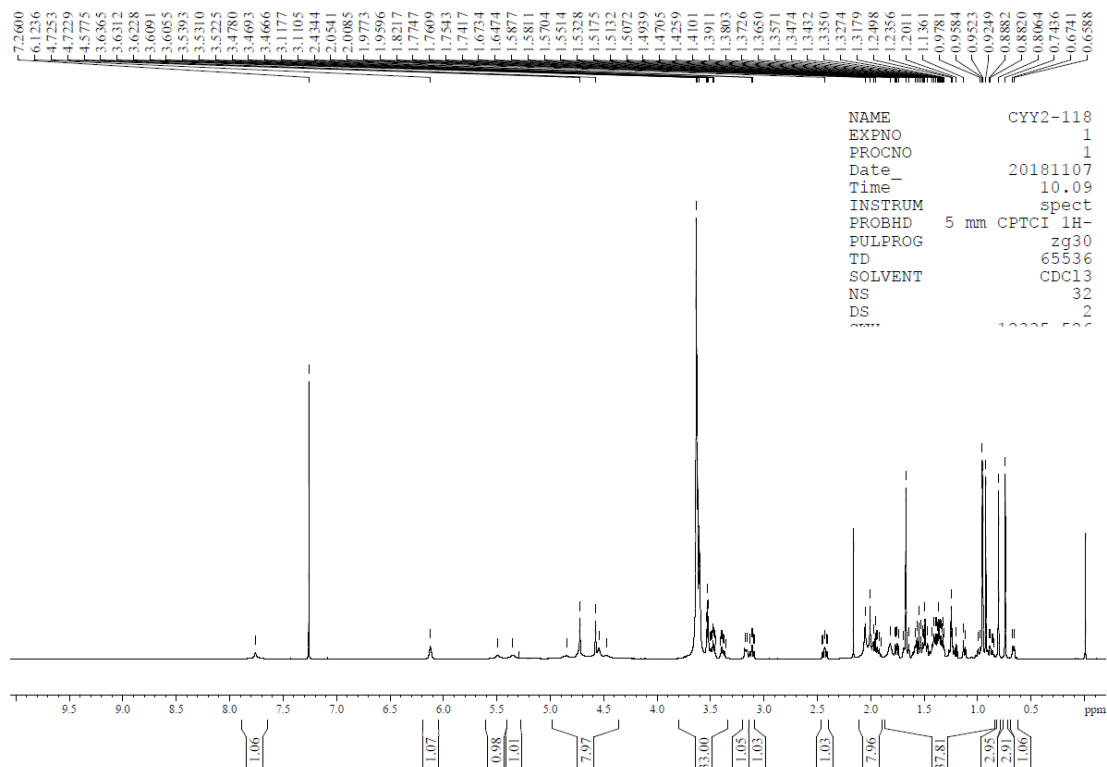
¹³C NMR of compound 66



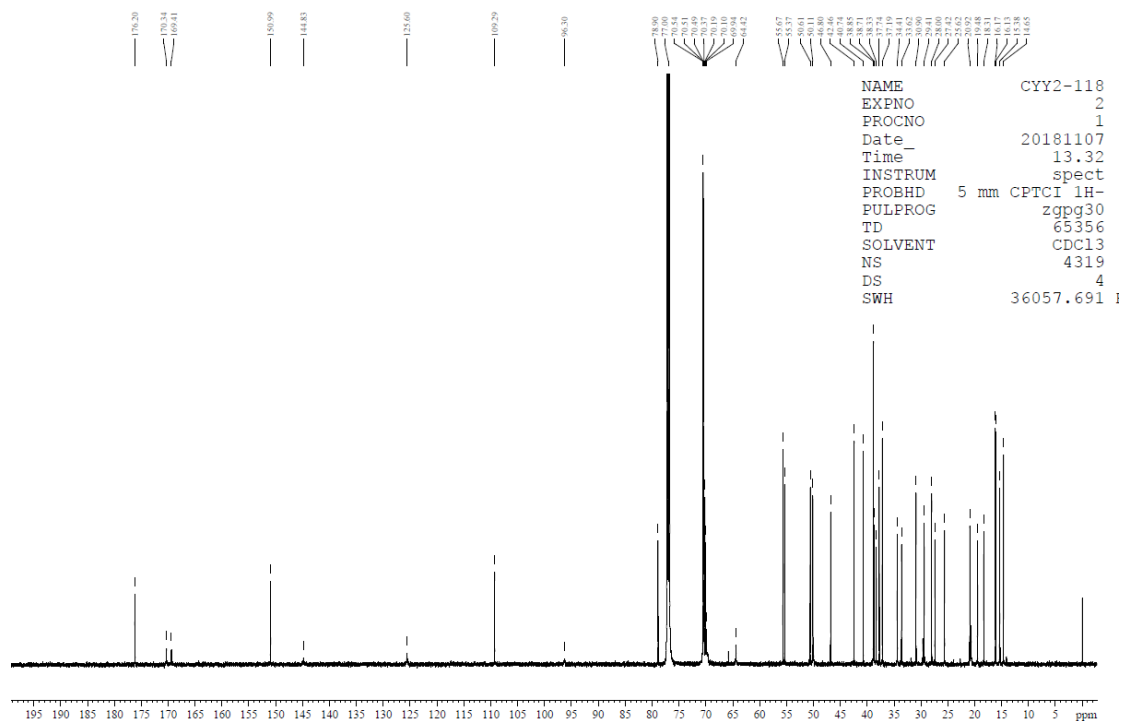
HRMS of compound **66**



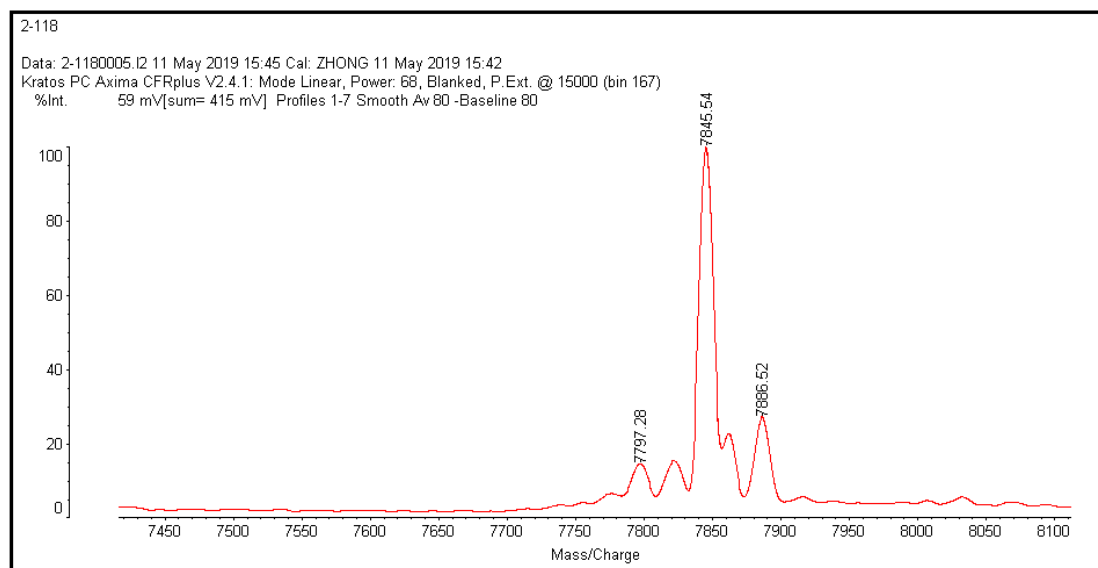
^1H NMR of compound **67**



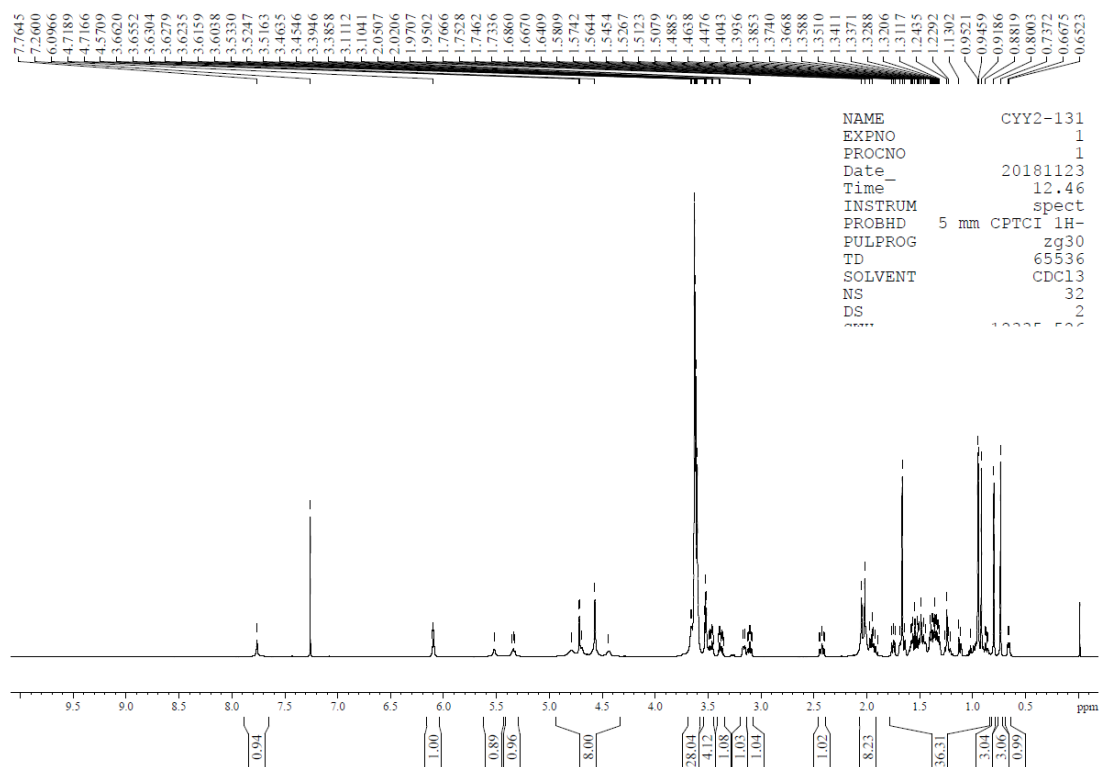
¹³C NMR of compound **67**



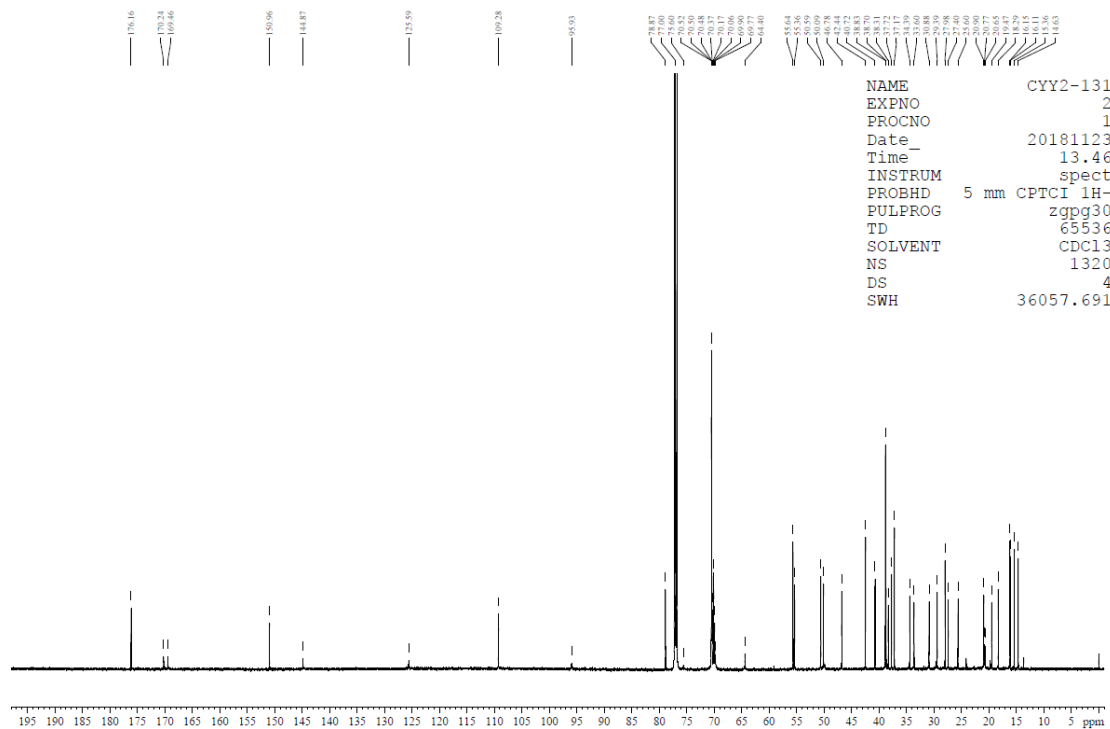
HRMS of compound **67**



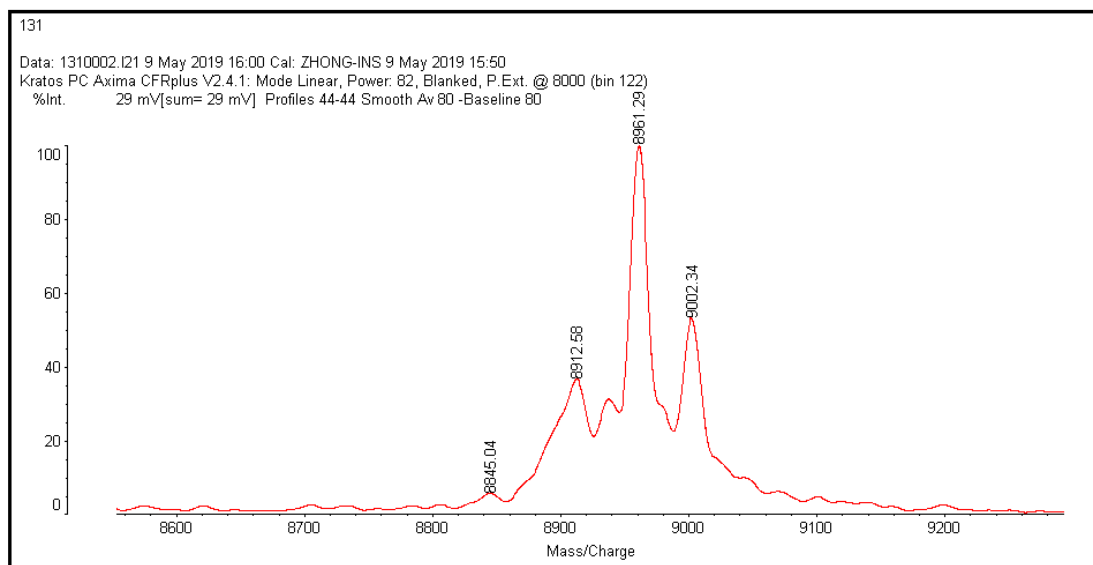
¹H NMR of compound 68



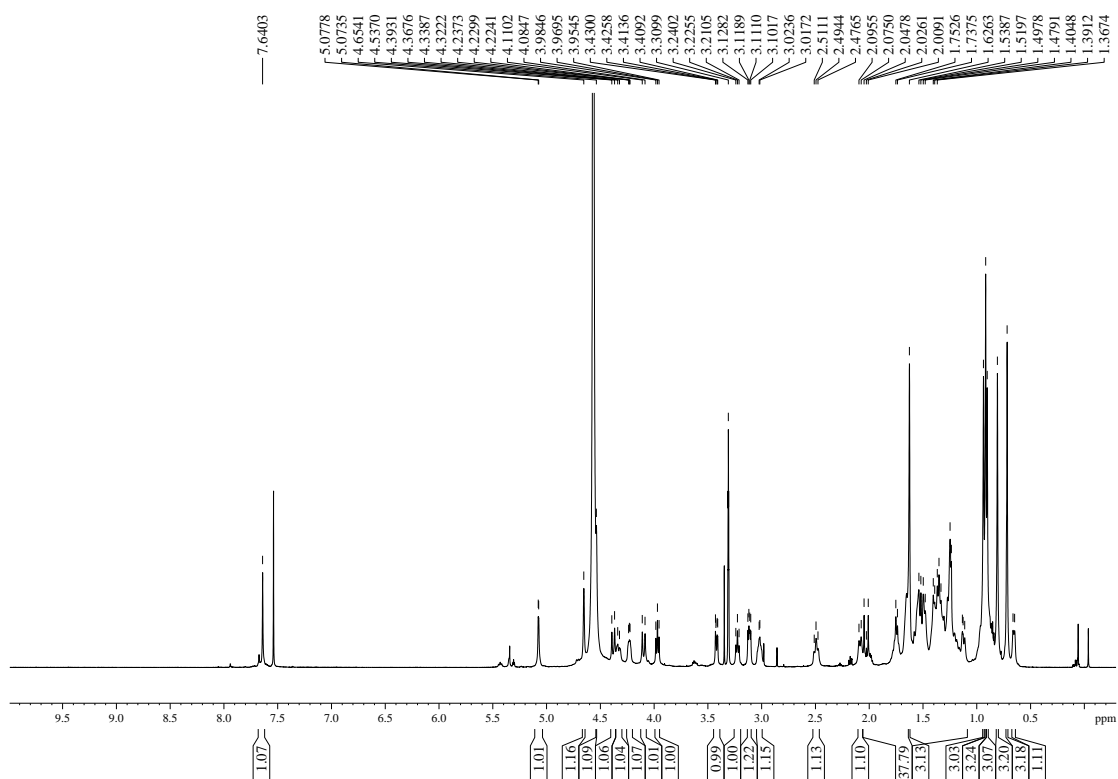
¹³C NMR of compound 68



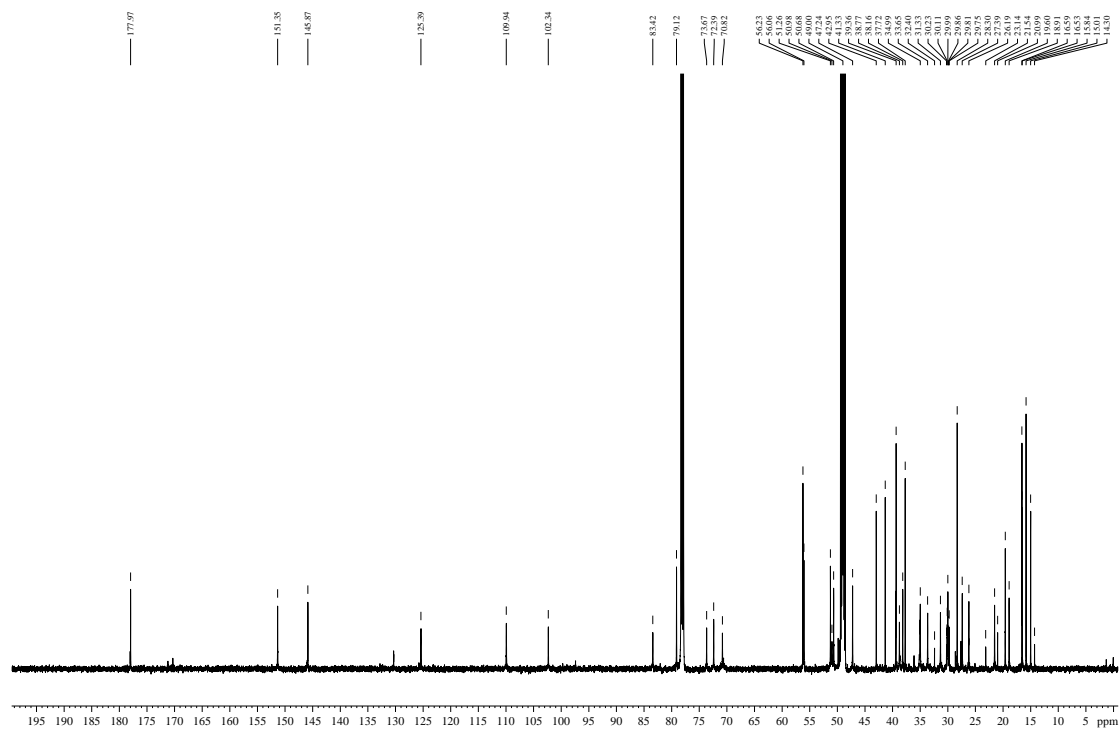
HRMS of compound **69**



^1H NMR of compound **69**

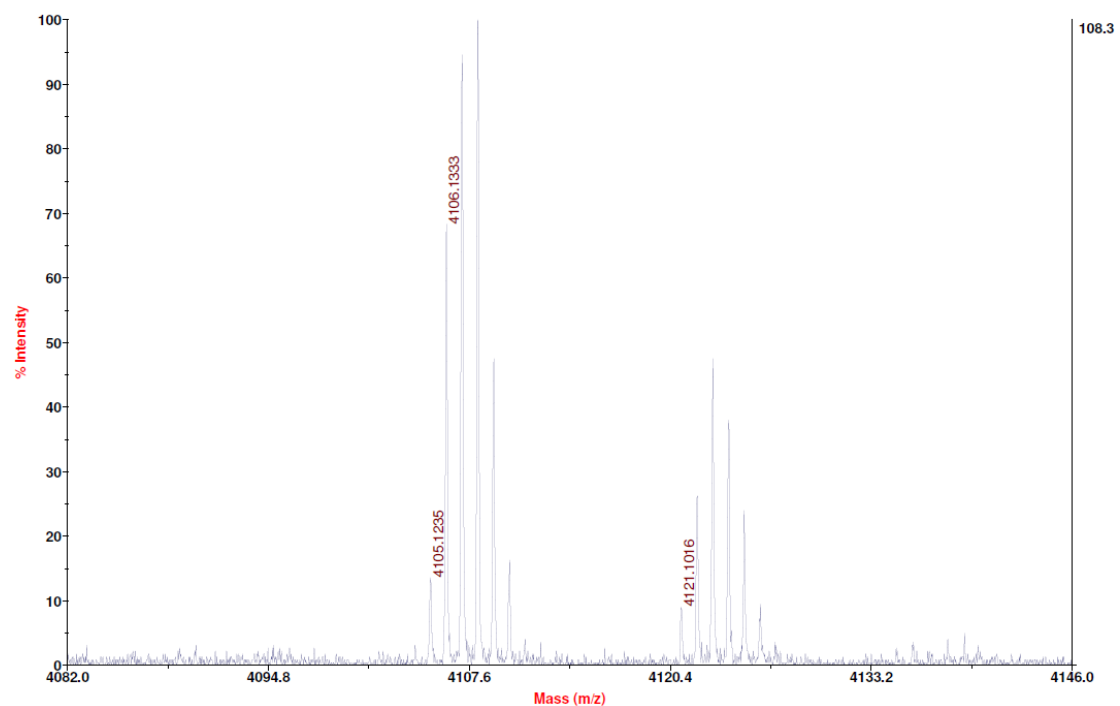


¹³C NMR of compound **69**

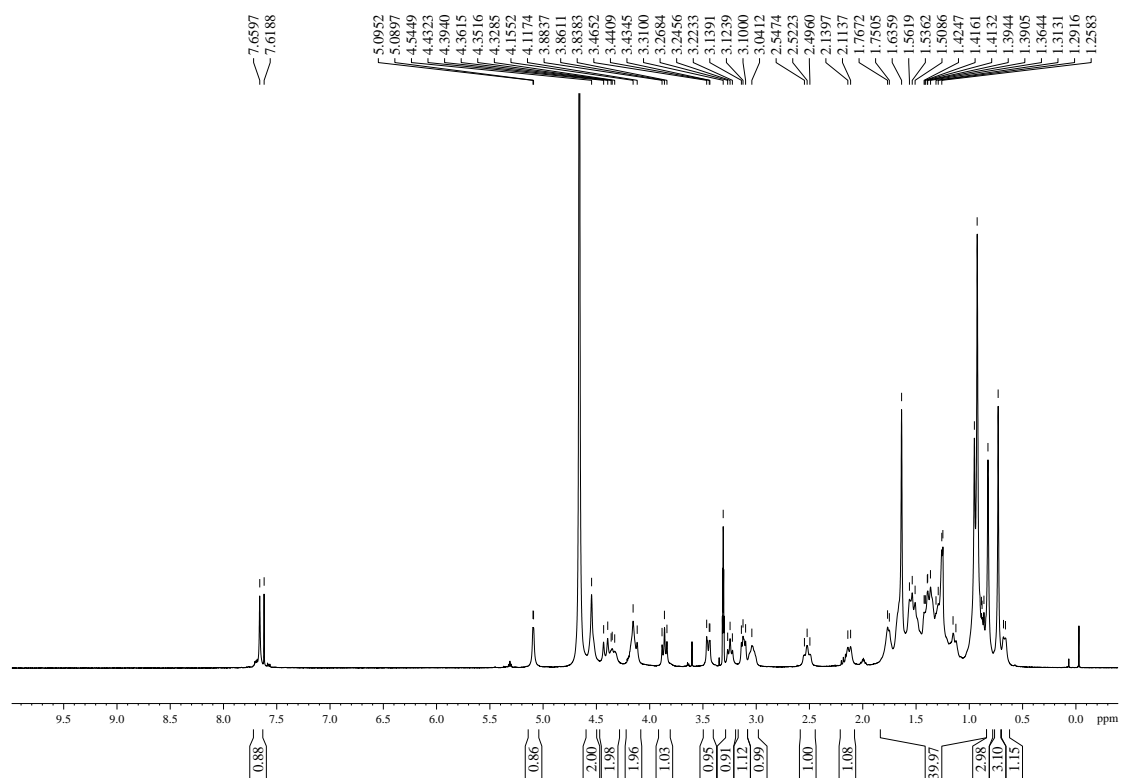


MALDI-TOF of compound **69**

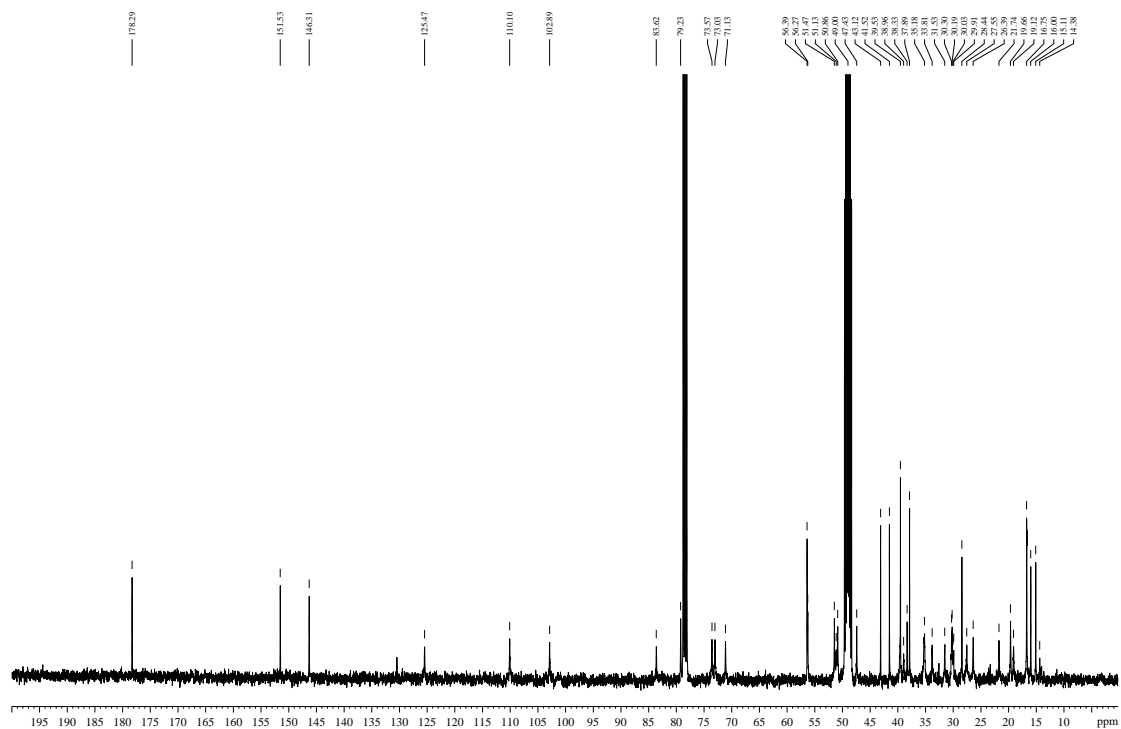
TOF/TOF™ Reflector Spec #1 MC[BP = 4108.1, 108]



¹H NMR of compound **70**

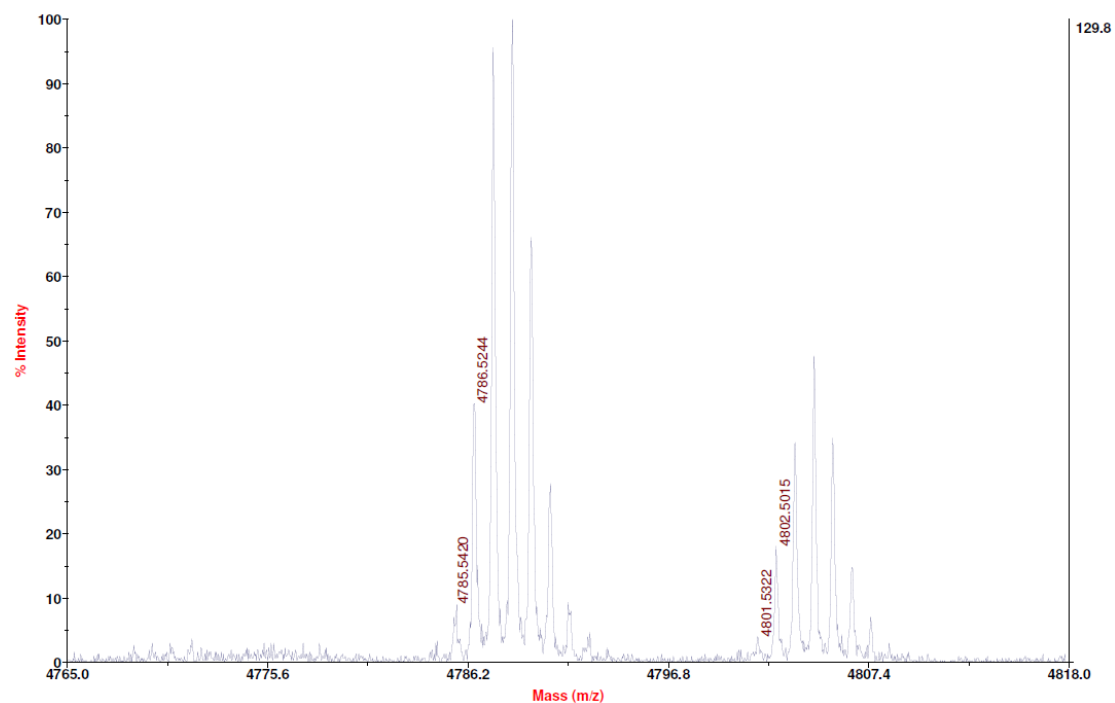


¹³C NMR of compound **70**

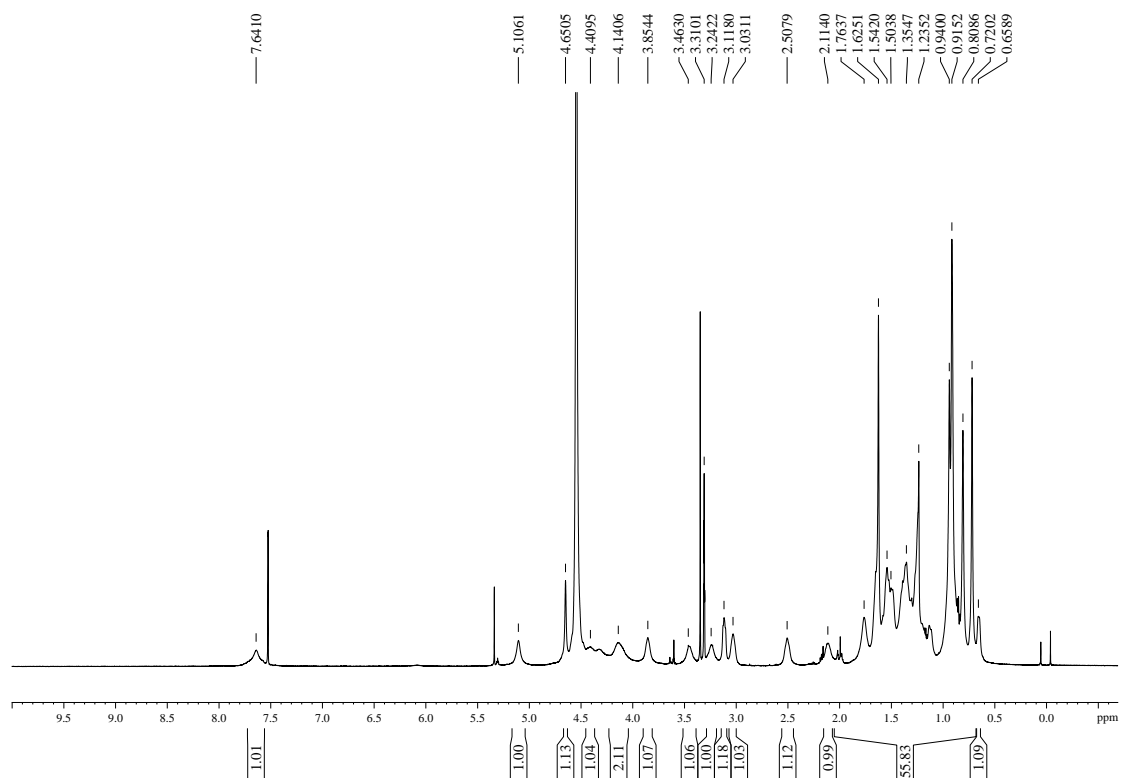


MALDI-TOF of compound **70**

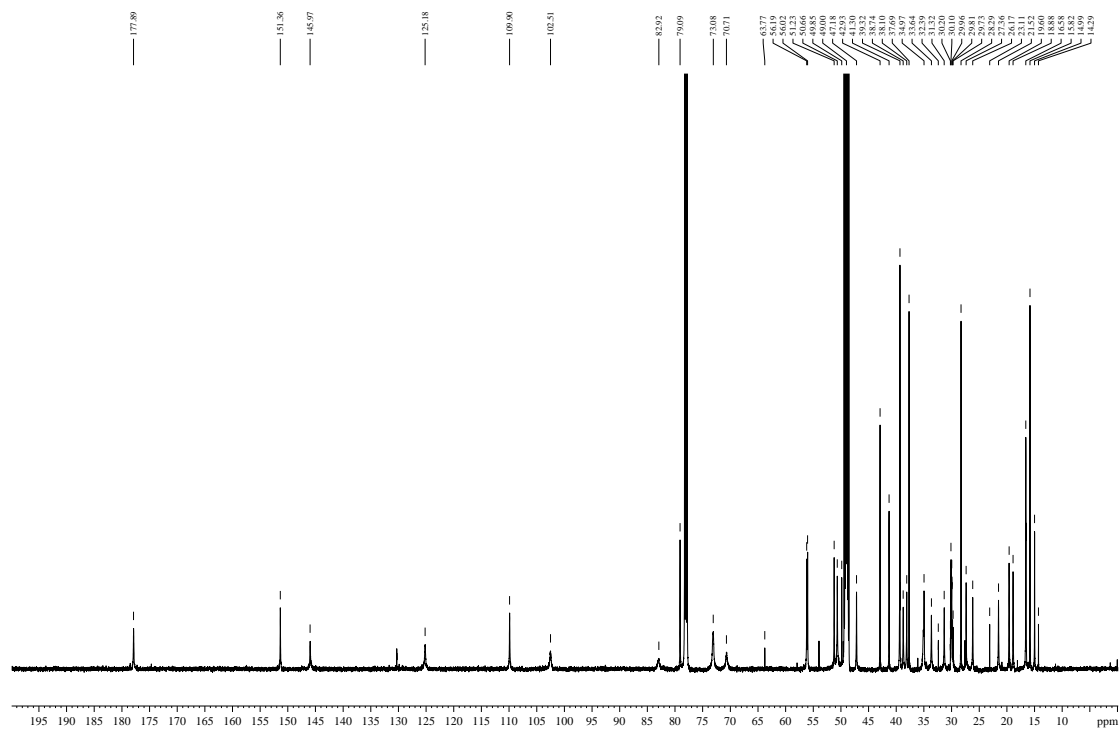
TOF/TOF™ Reflector Spec #1 MC[BP = 1081.9, 307]



¹H NMR of compound **71**

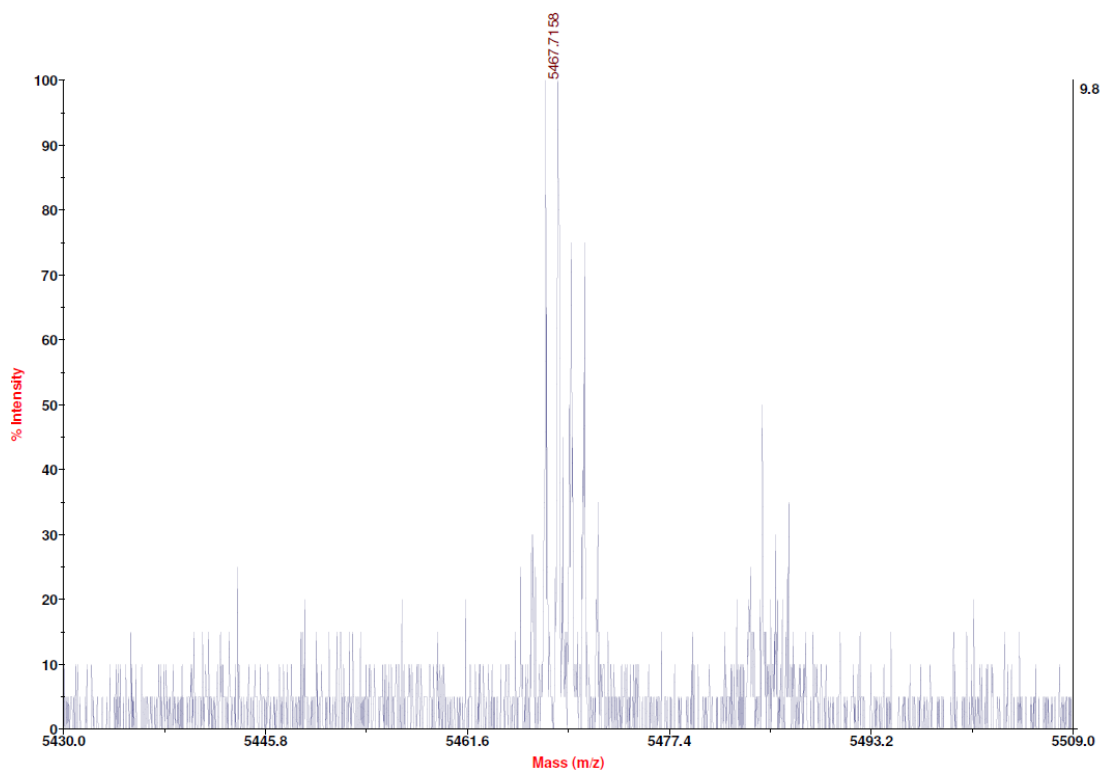


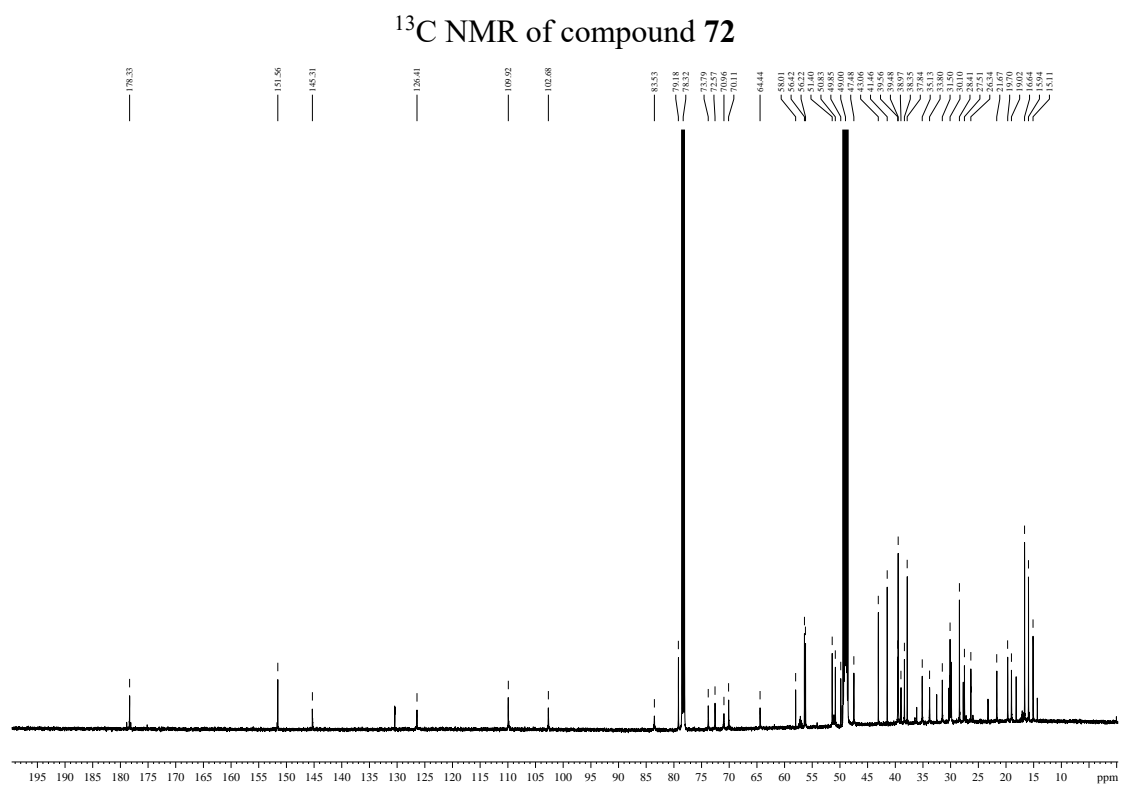
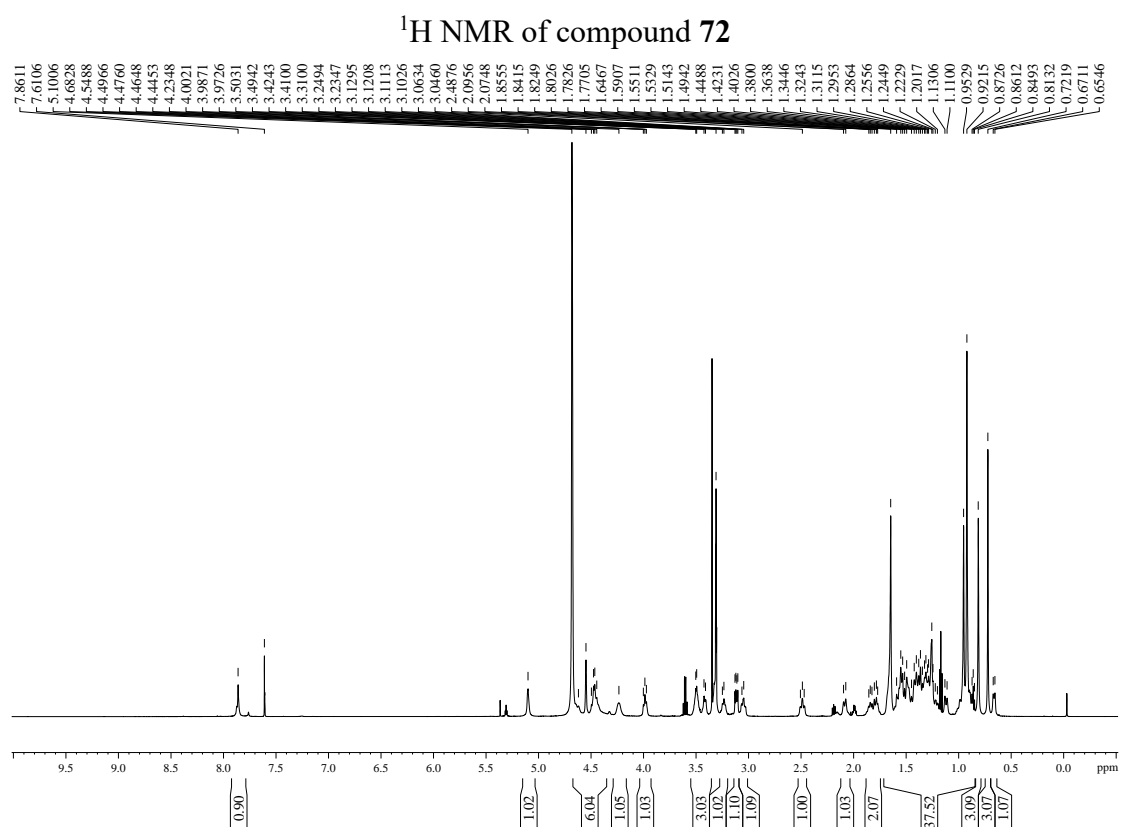
¹³C NMR of compound **71**



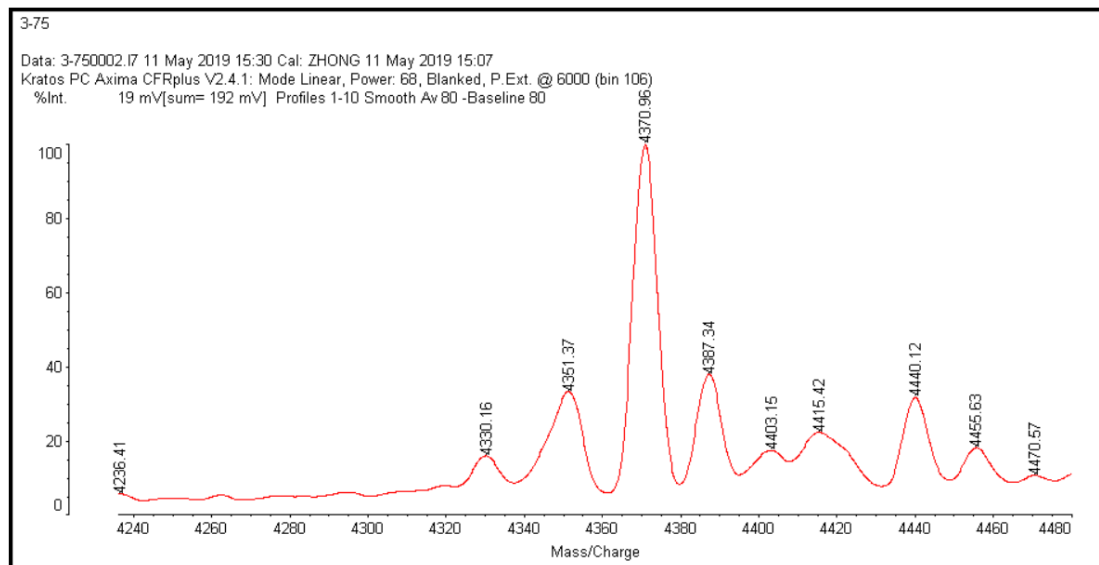
MALDI-TOF of compound **71**

TOF/TOF™ Reflector Spec #1 MC[BP = 1081.9, 216]

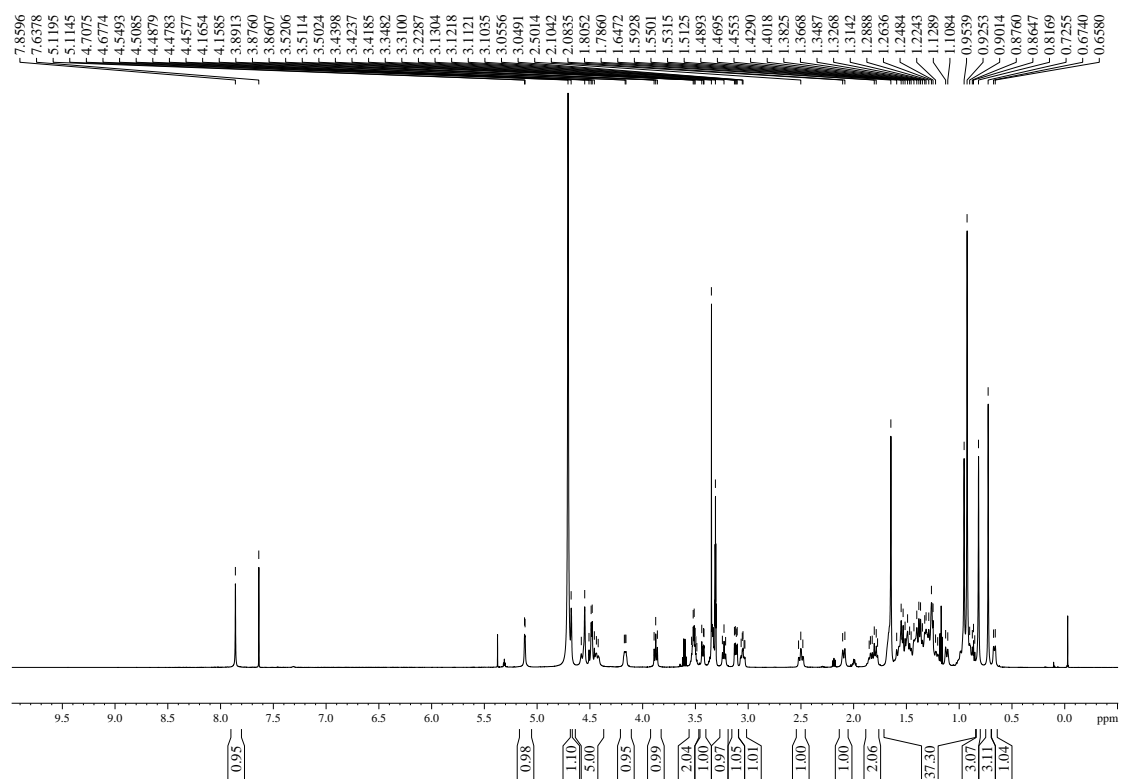




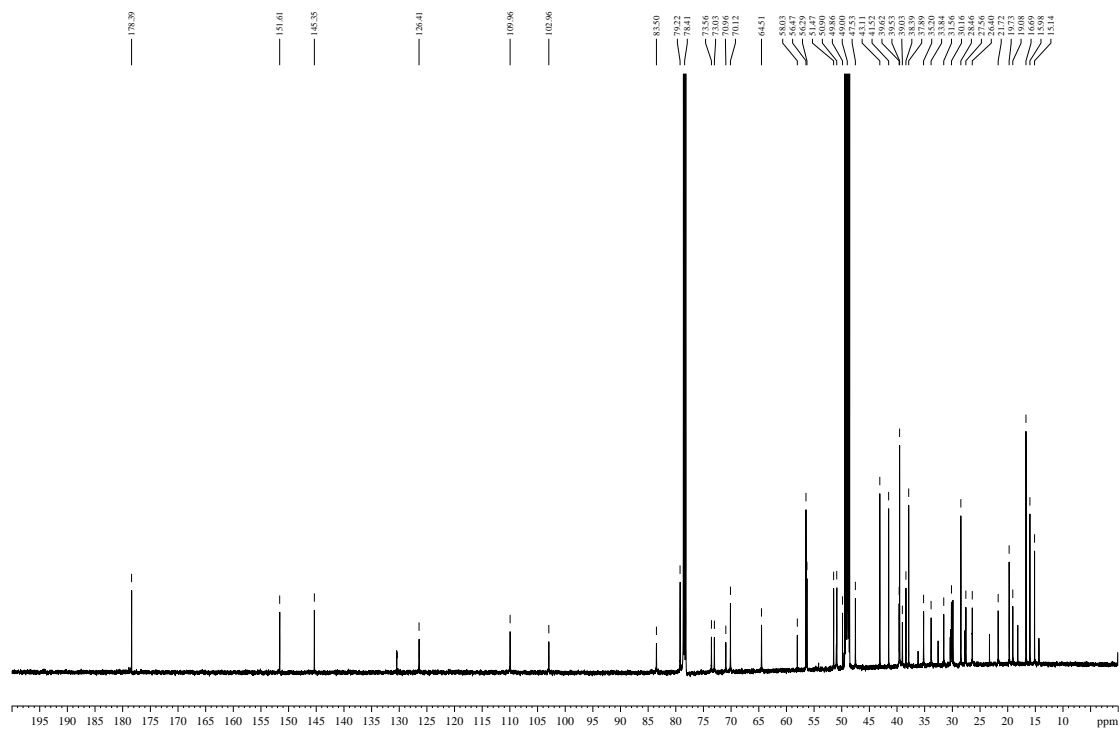
MALDI-TOF of compound **72**



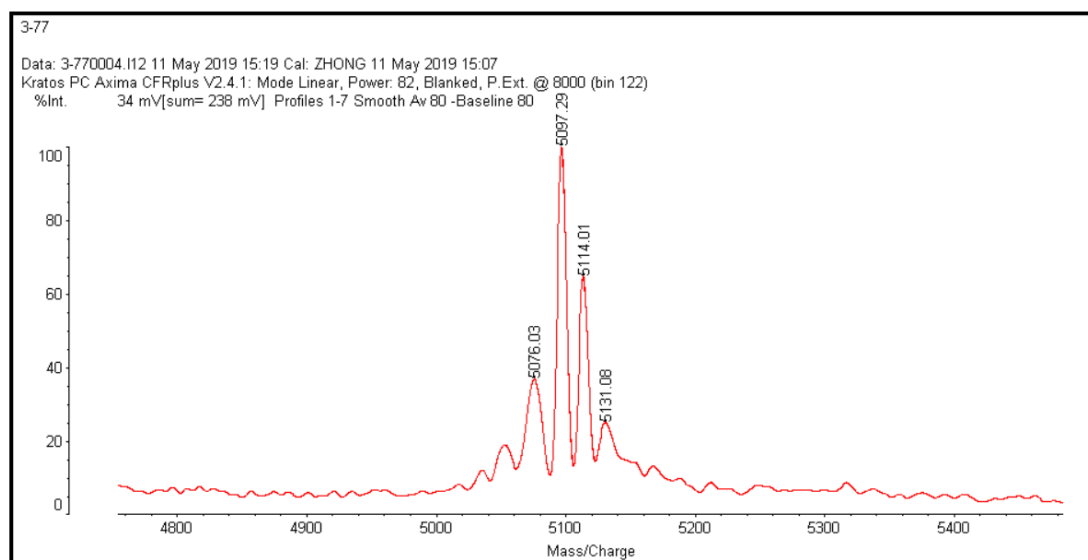
^1H NMR of compound **73**

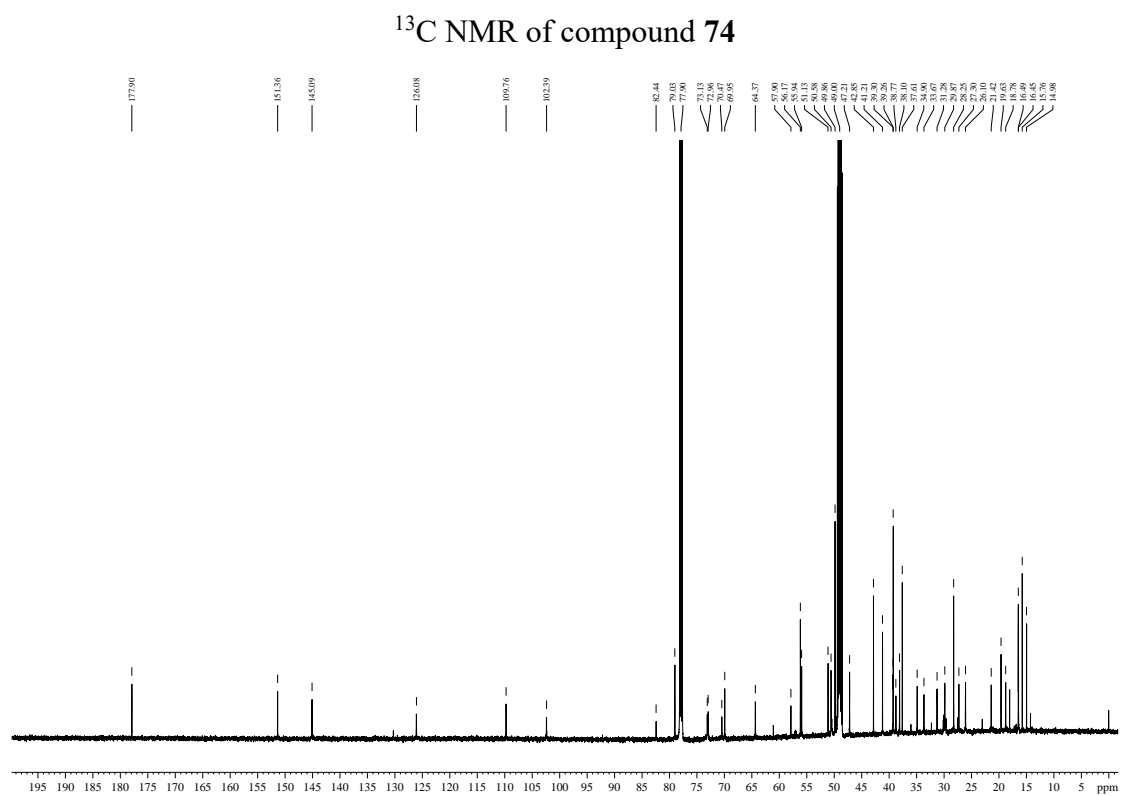
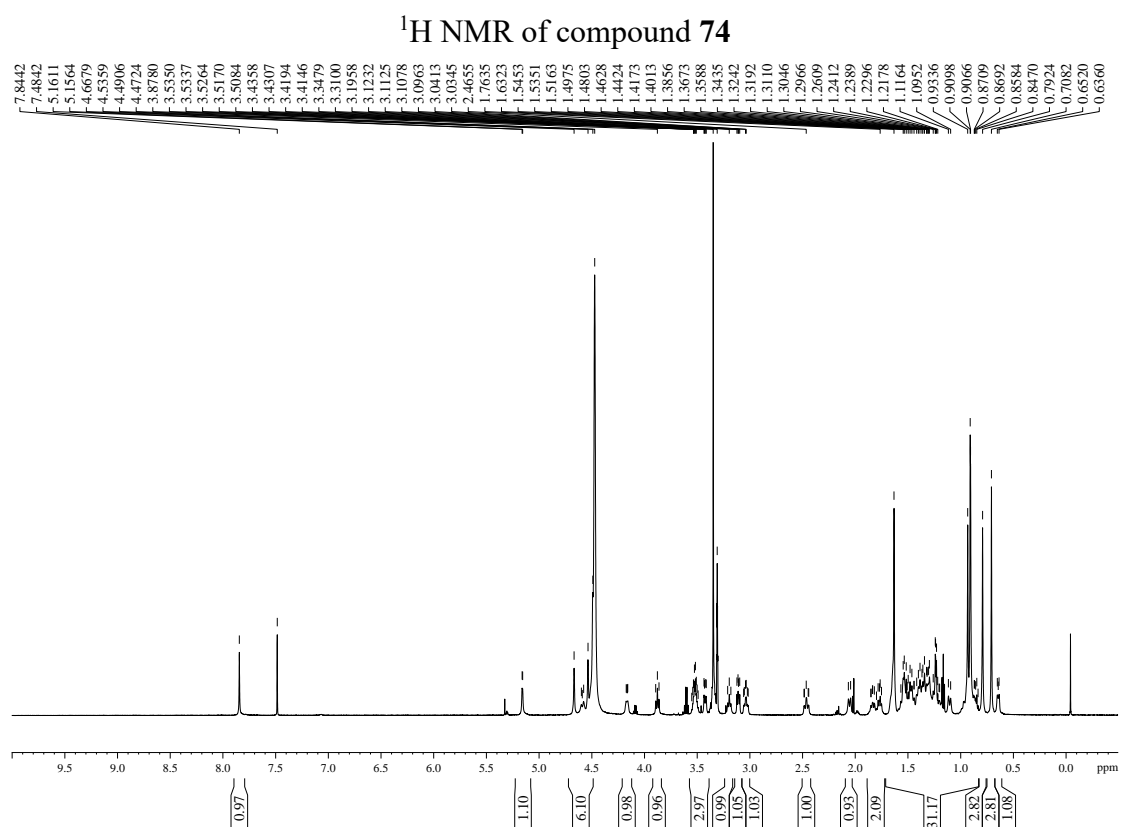


^{13}C NMR of compound **73**

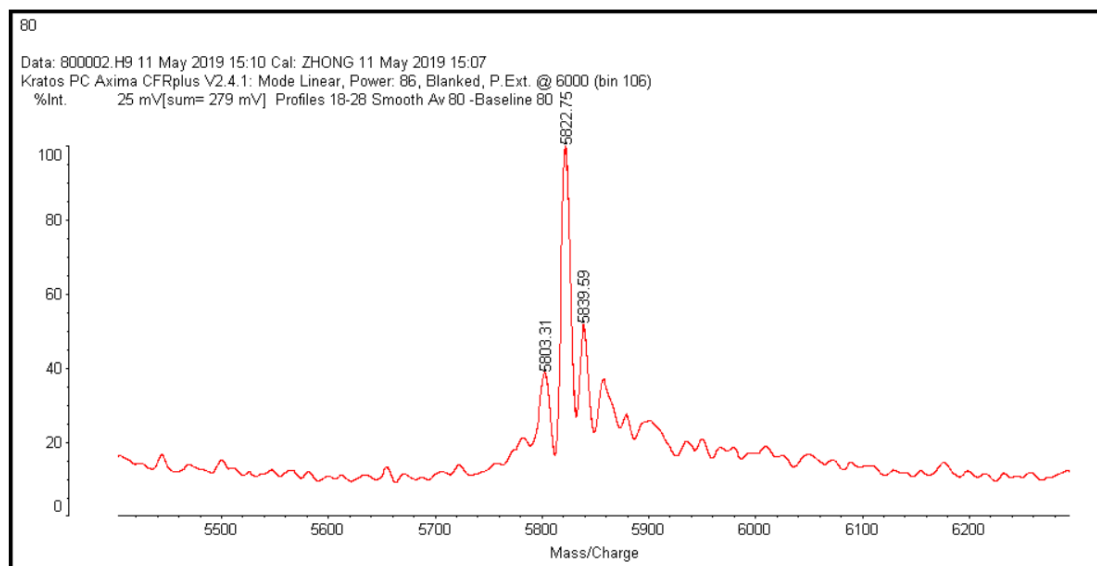


MALDI-TOF of compound **73**

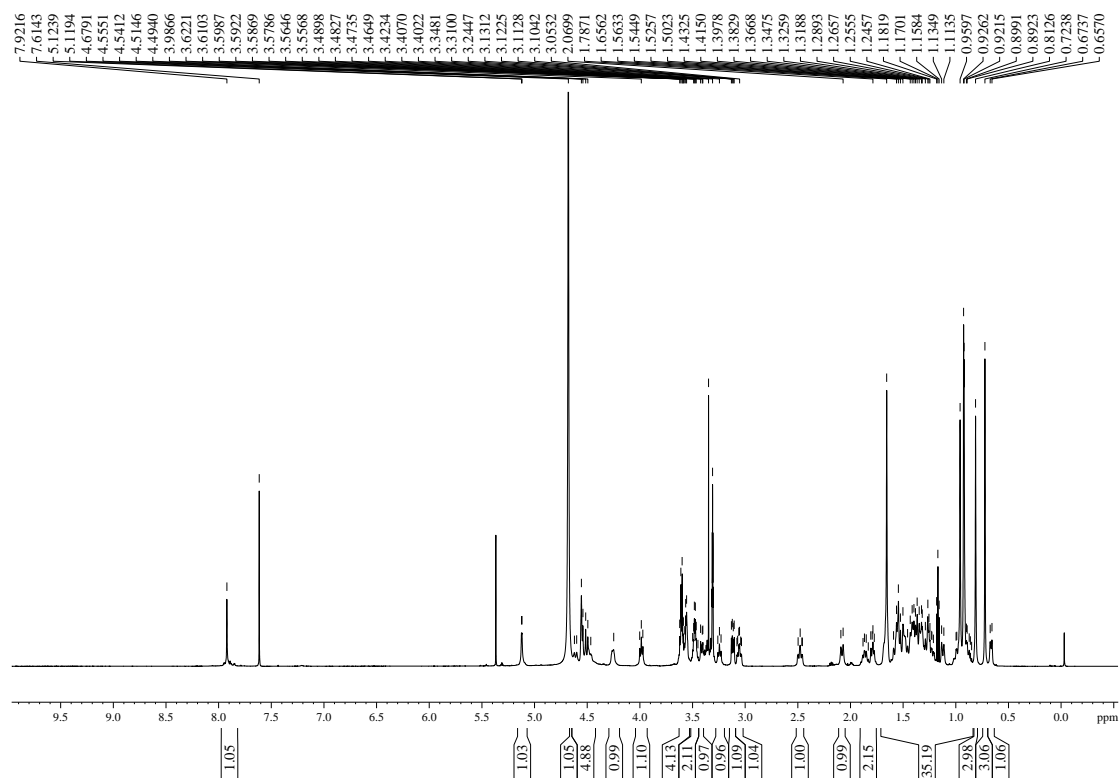




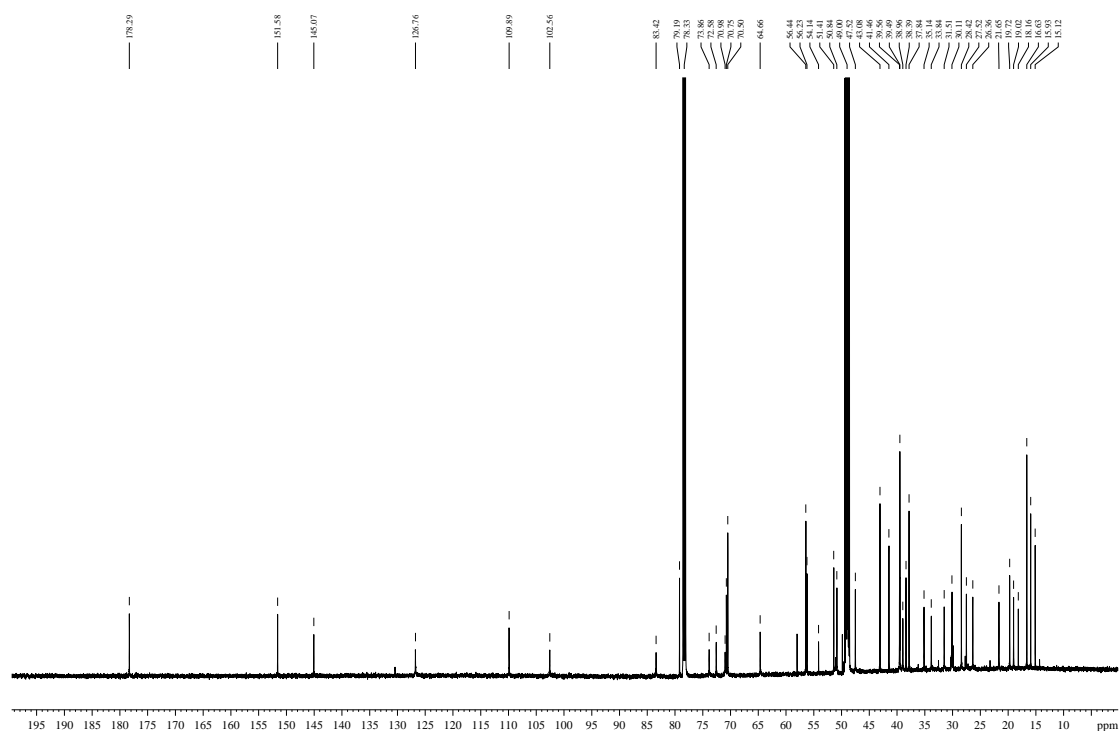
MALDI-TOF of compound **74**



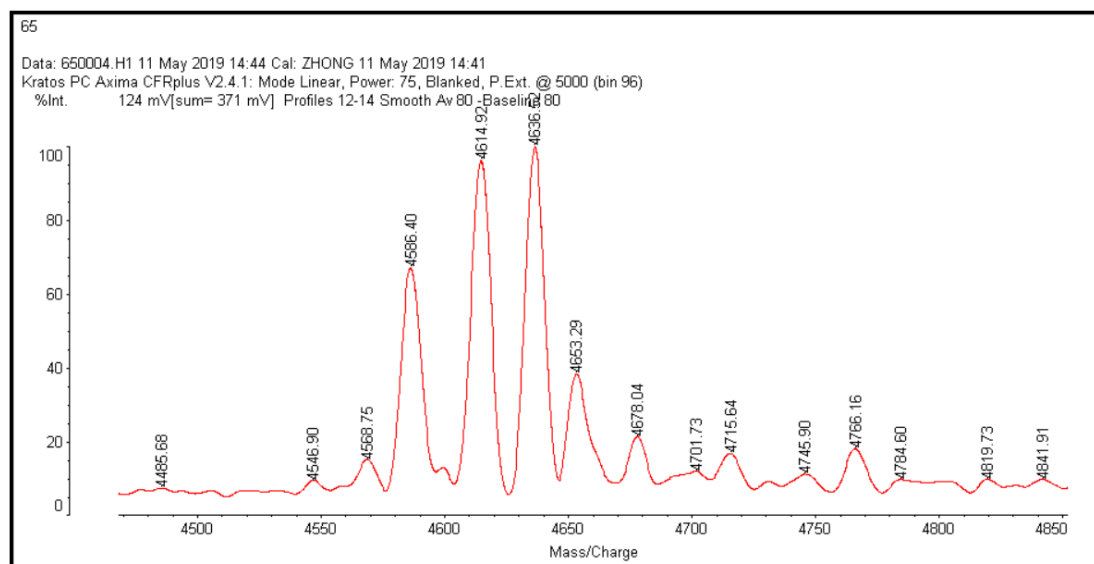
¹H NMR of compound **75**

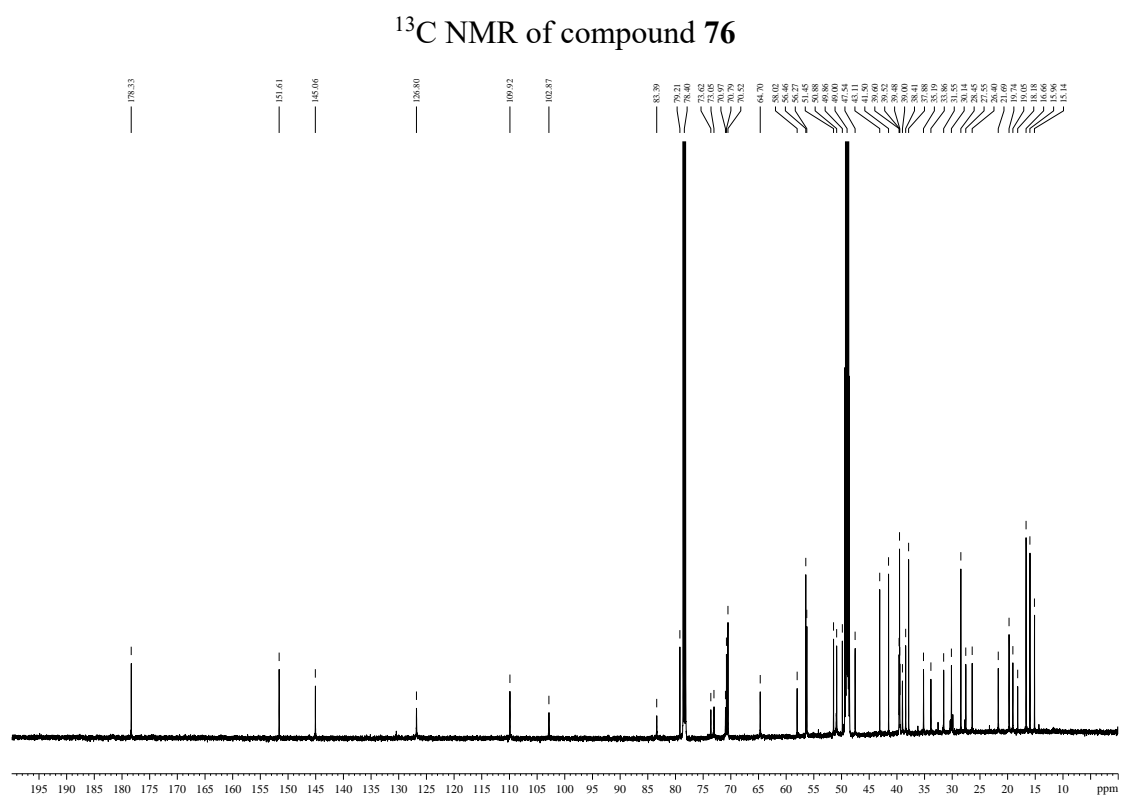
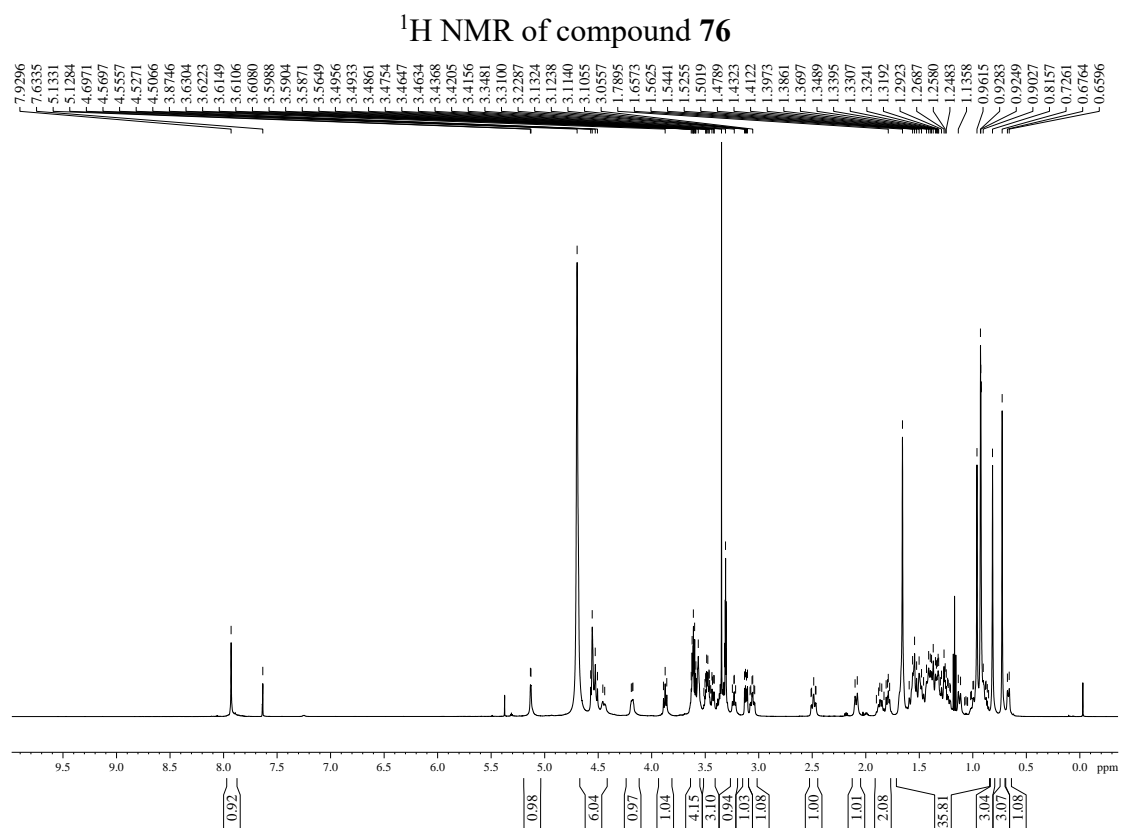


¹³C NMR of compound **75**

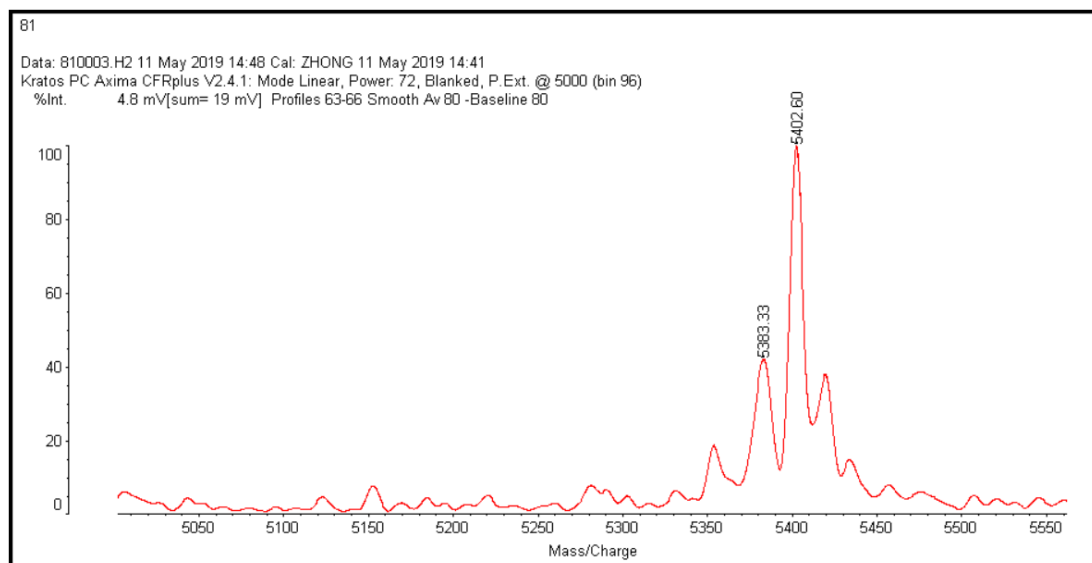


MALDI-TOF of compound **75**

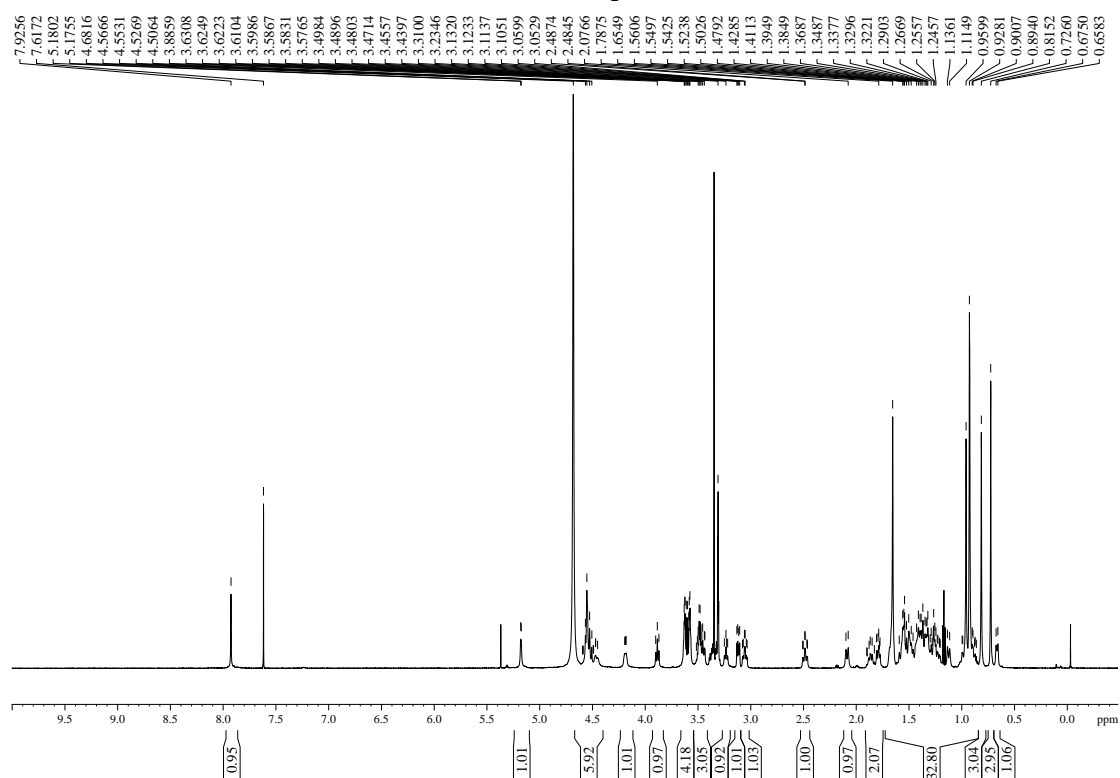




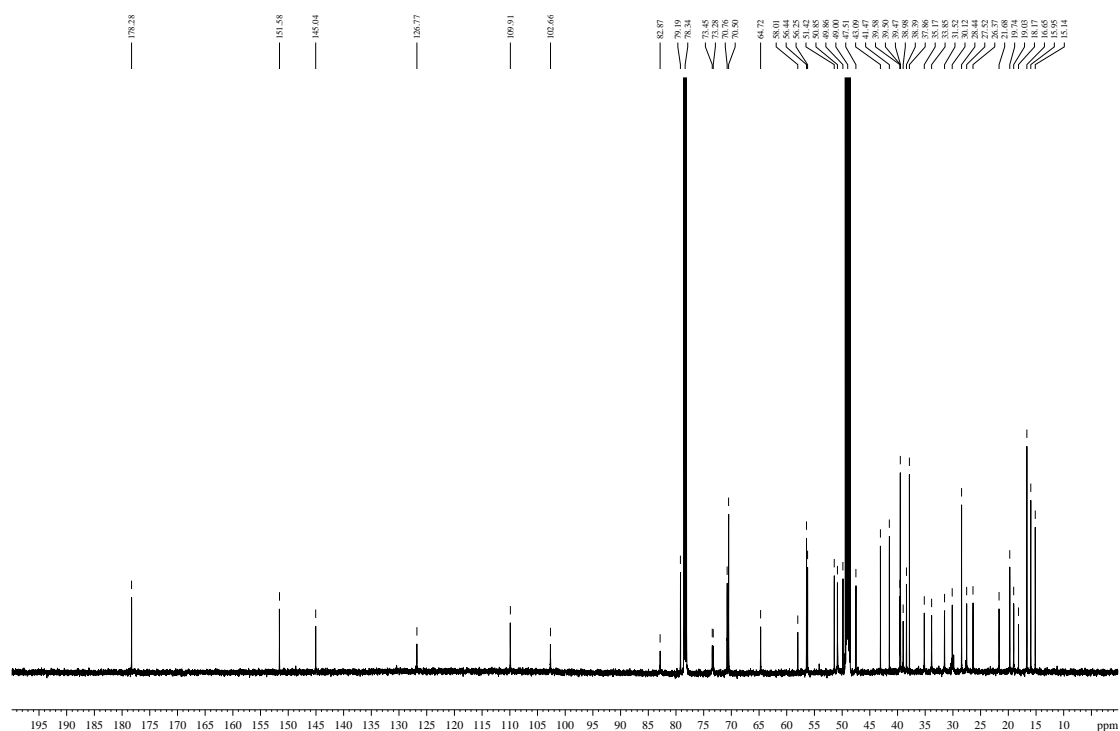
MALDI-TOF of compound 76



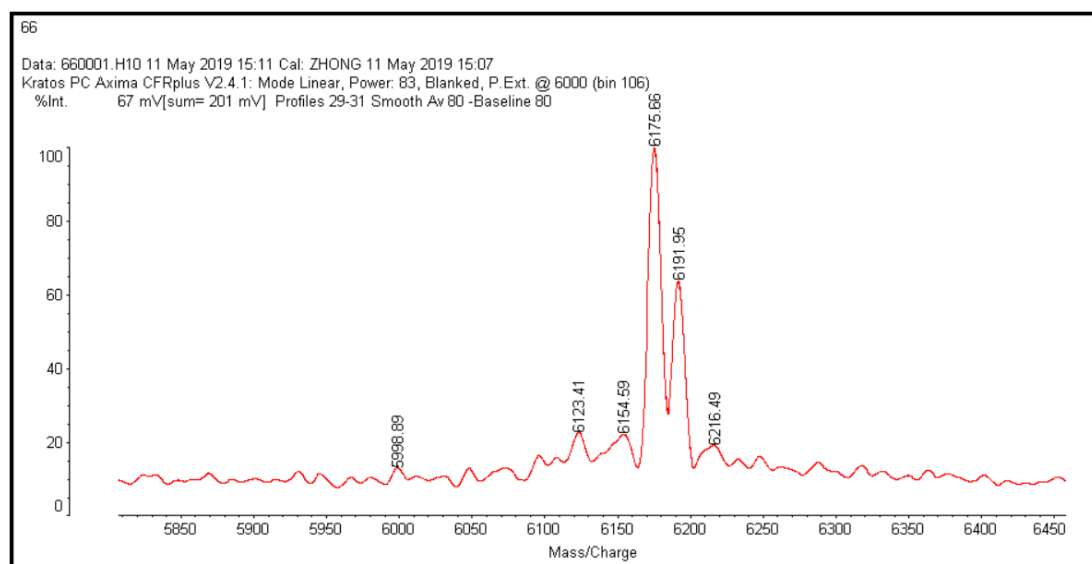
¹H NMR of compound 77



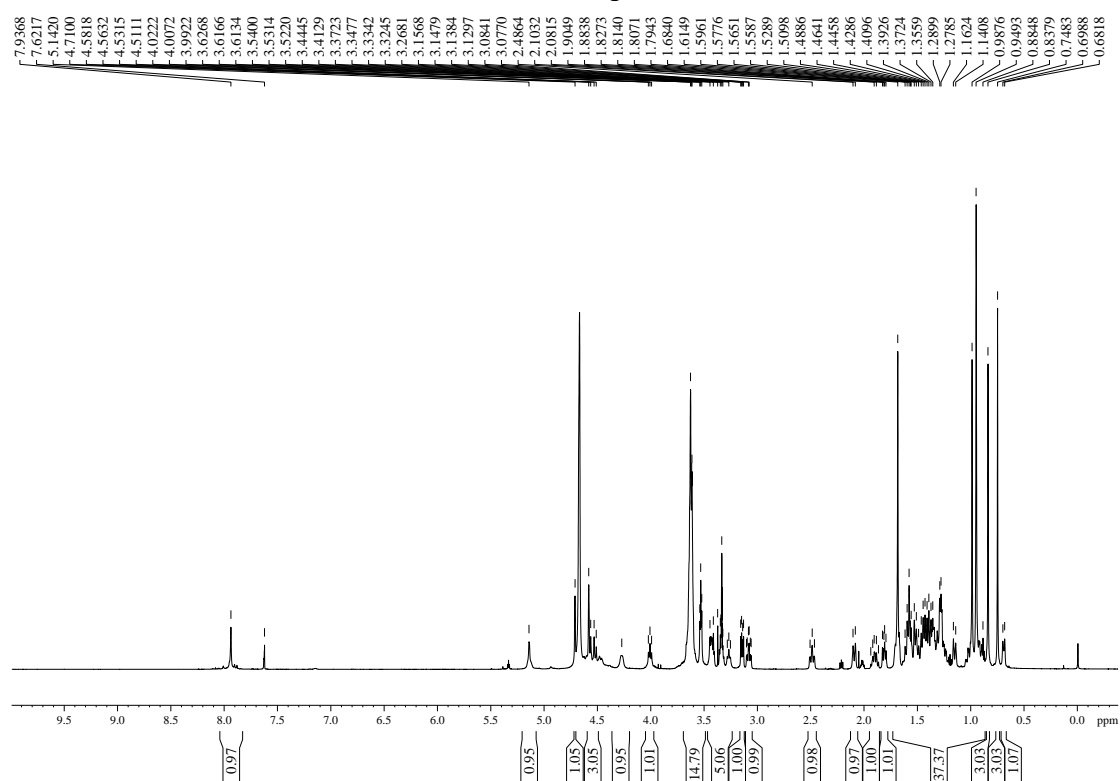
¹³C NMR of compound 77



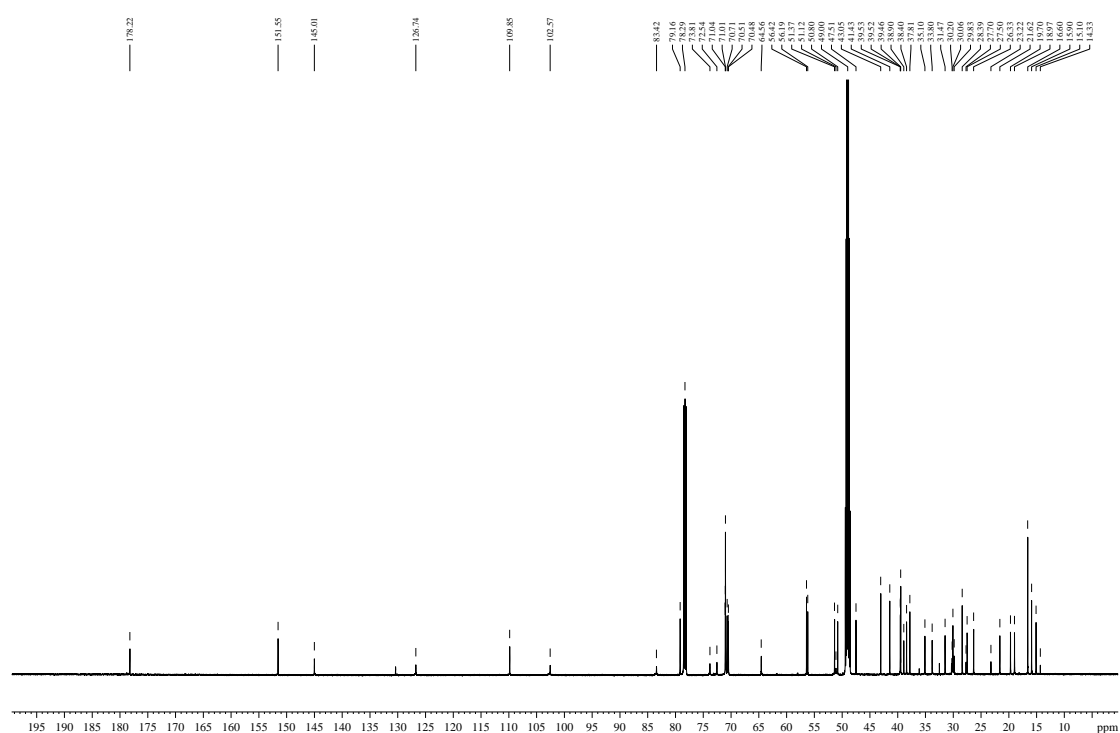
MALDI-TOF of compound 77



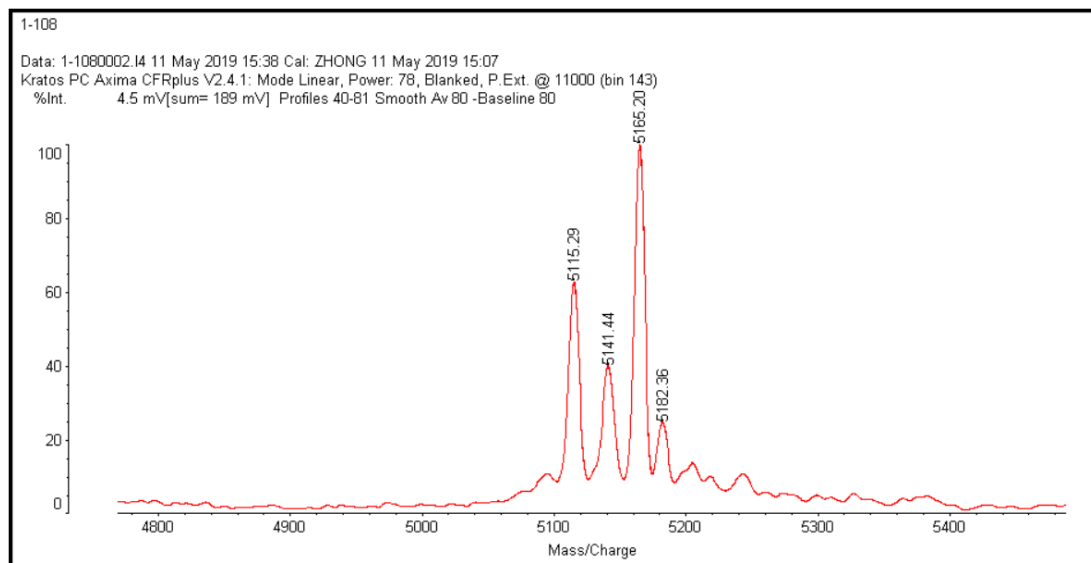
¹H NMR of compound 78



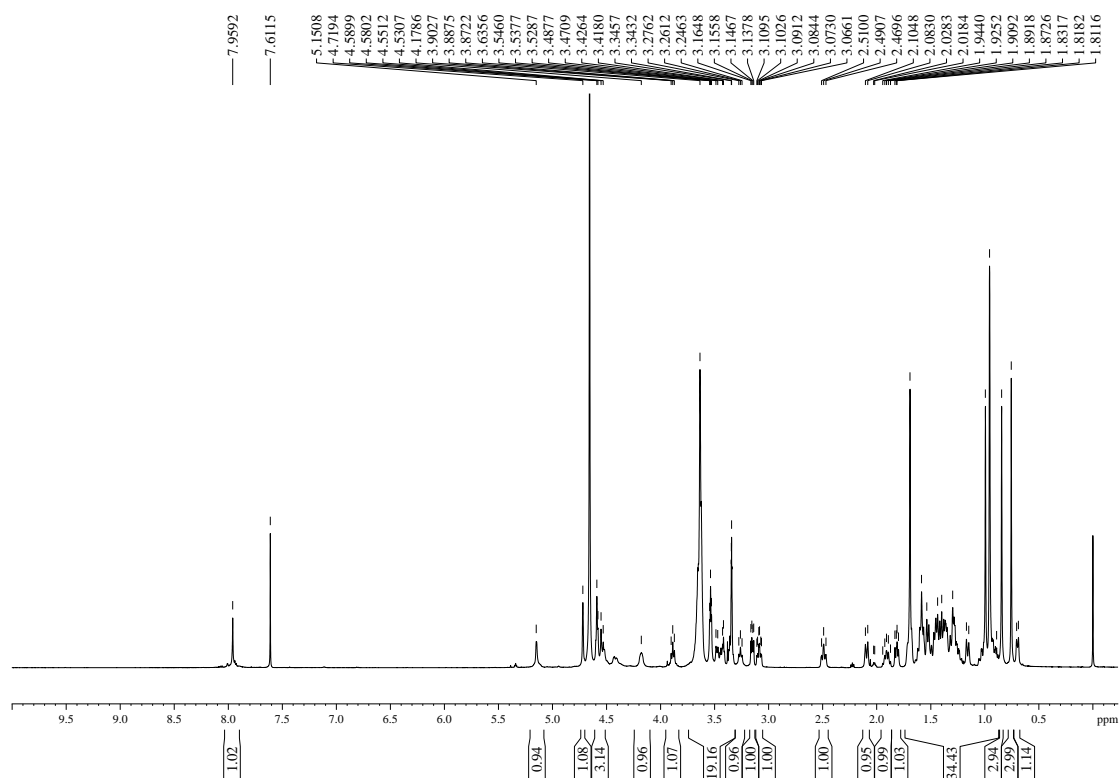
¹³C NMR of compound 78



MALDI-TOF of compound 78



¹H NMR of compound 79

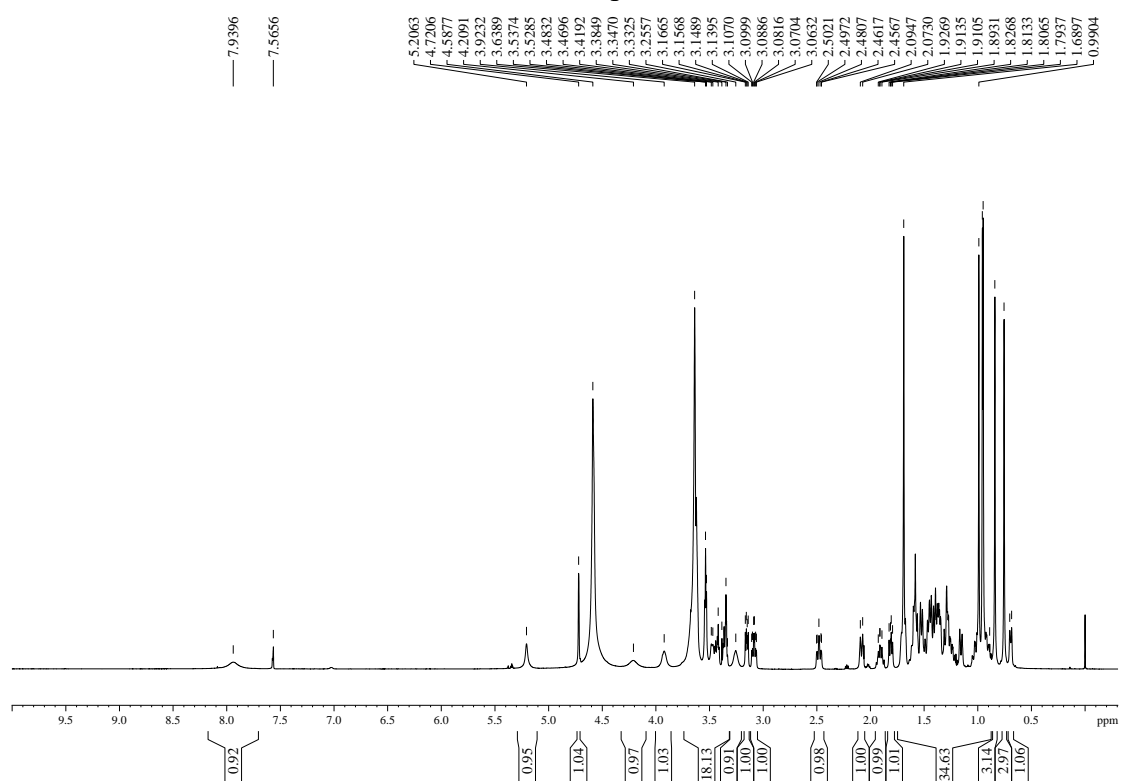


1-110

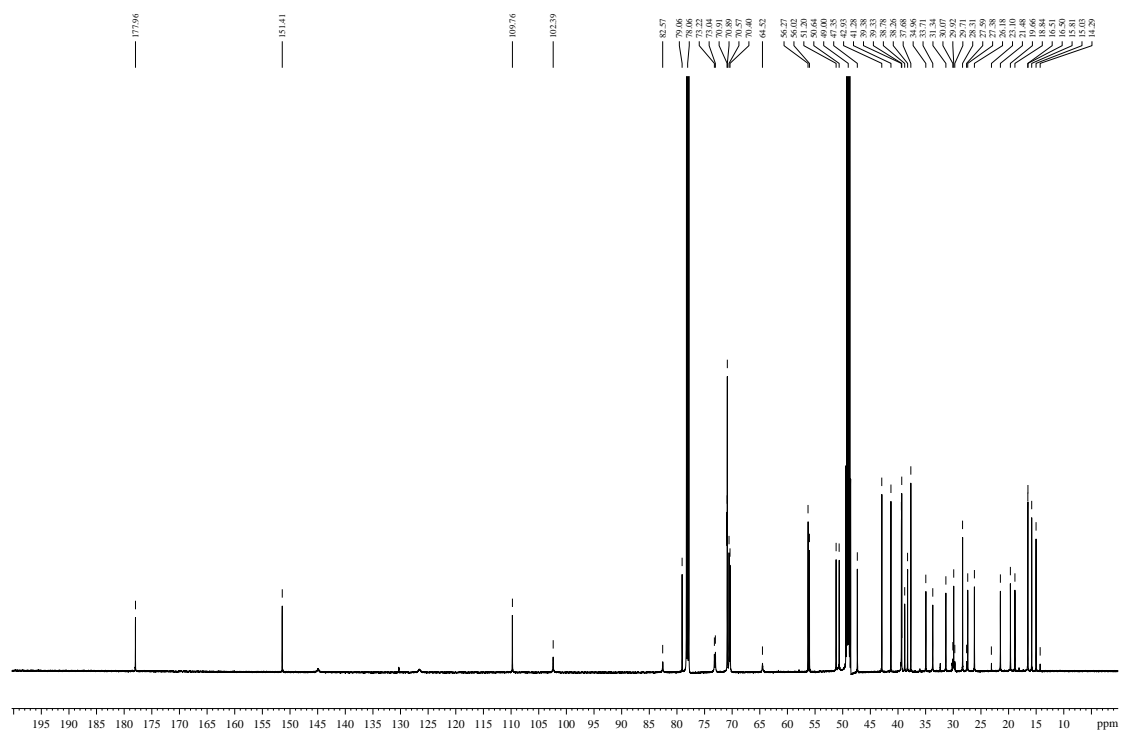
Data: 1100002.H3 11 May 2019 14:52 Cal: ZHONG 11 May 2019 14:41
Kratos PC Axima CFRplus V2.4.1: Mode Linear, Power: 77, Blanked, P.Ext. @ 5000 (bin 96)
%Int. 20 mV[sum= 80 mV] Profiles 1-4 Smooth Av 80 -Baseline 80

Mass/Charge

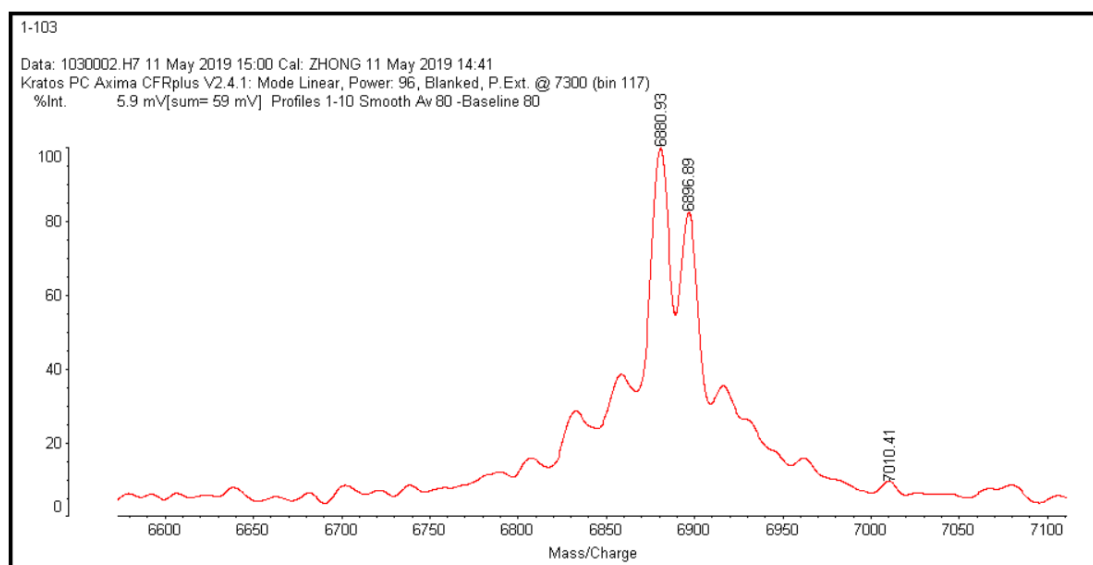
¹H NMR of compound **80**



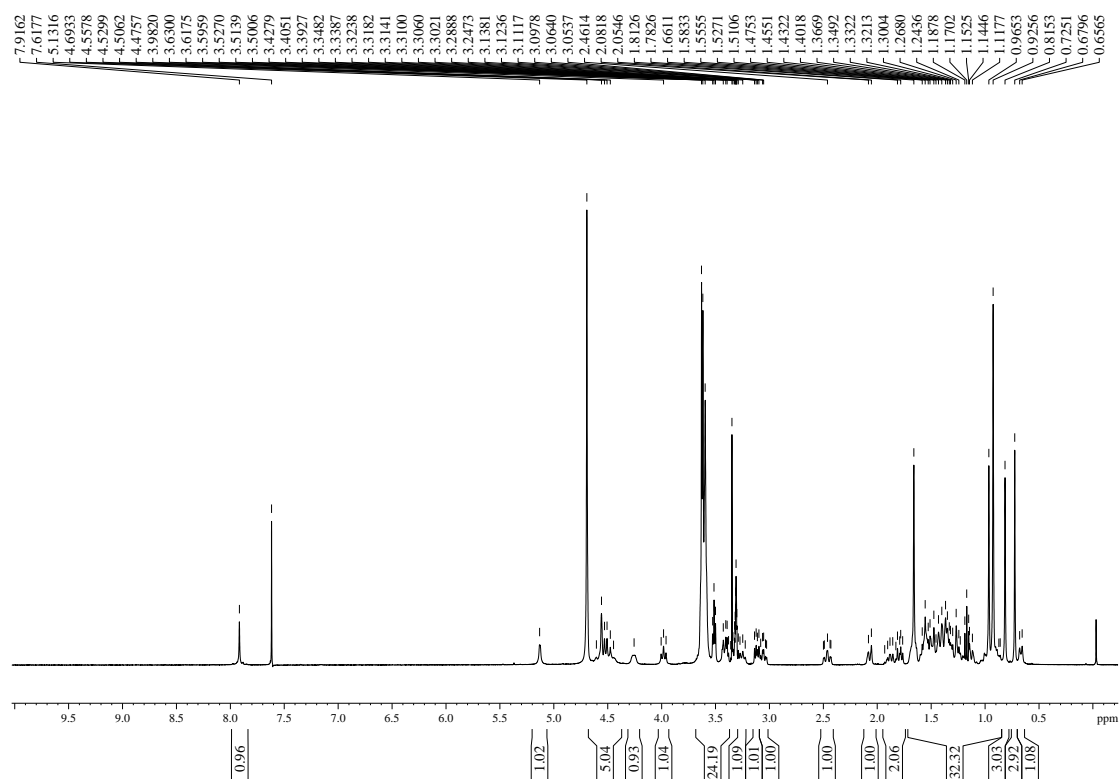
¹³C NMR of compound **80**



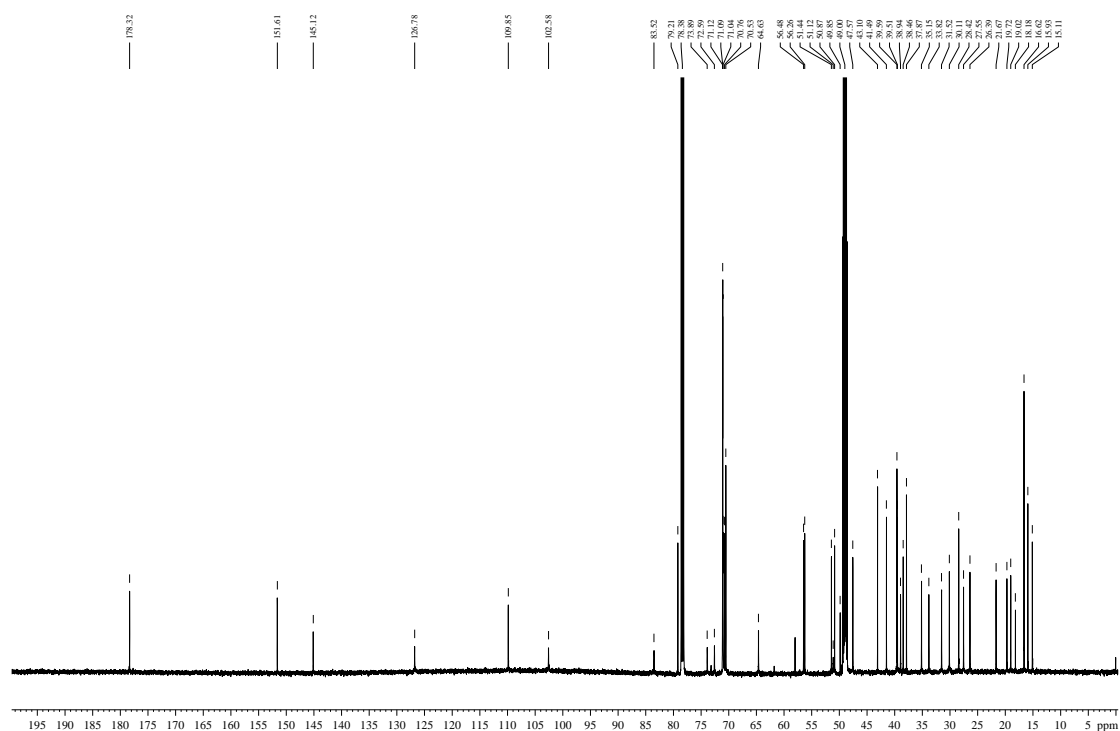
MALDI-TOF of compound **80**



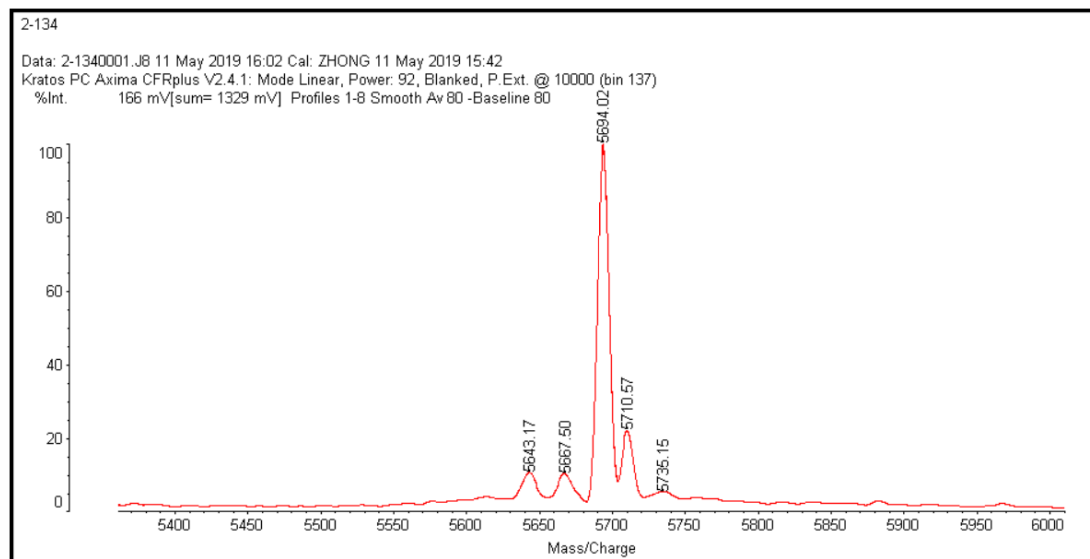
^1H NMR of compound **81**



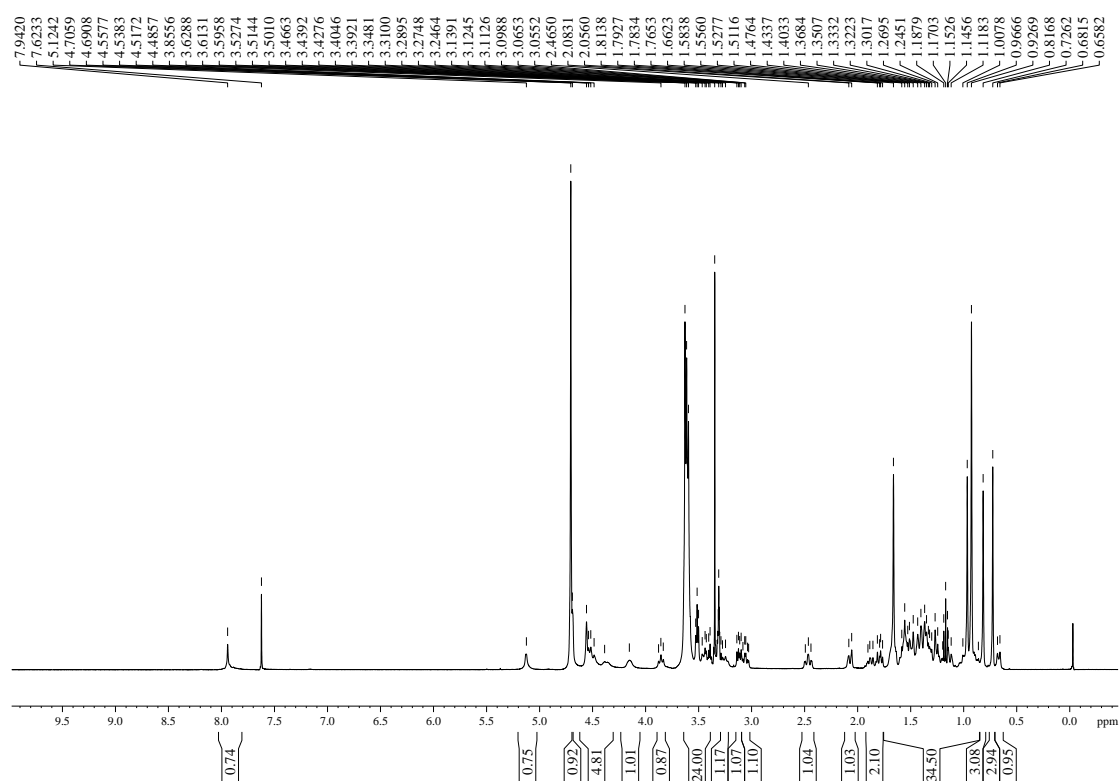
¹³C NMR of compound **81**



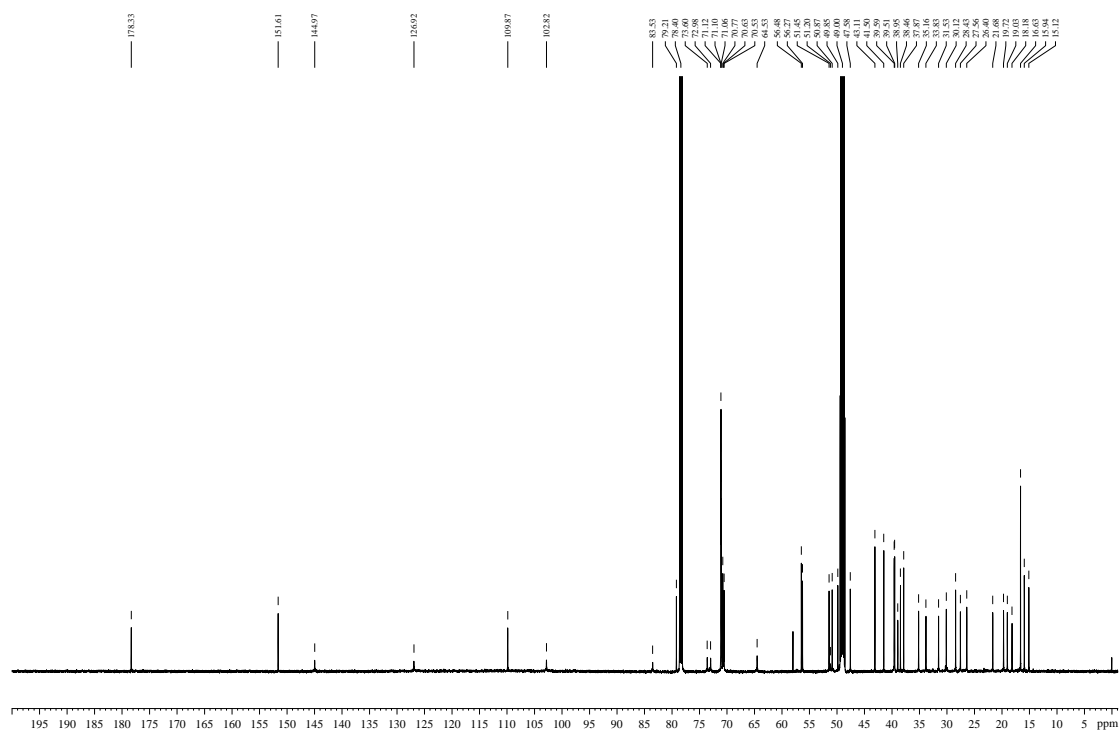
MALDI-TOF of compound **81**



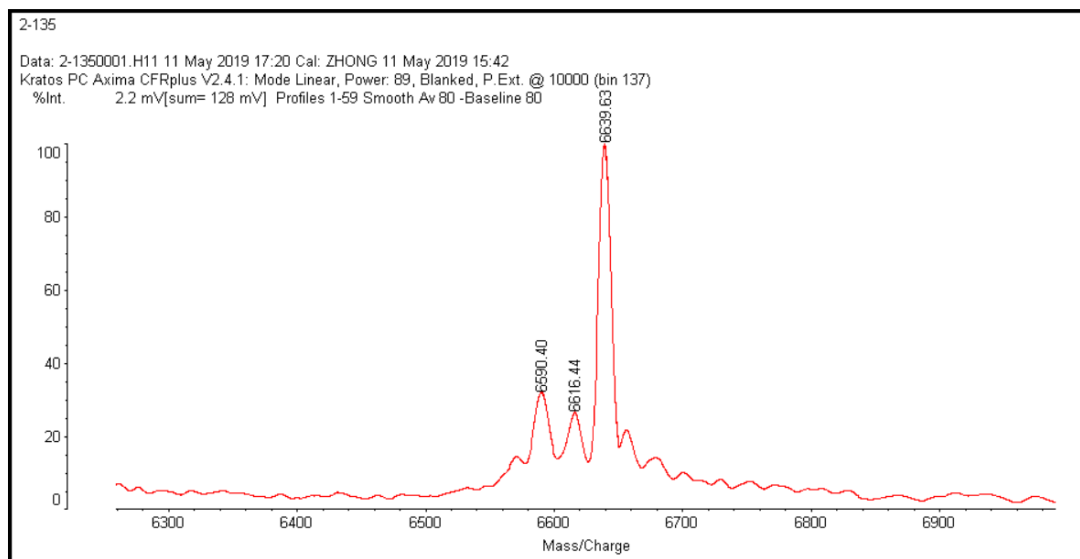
¹H NMR of compound **82**



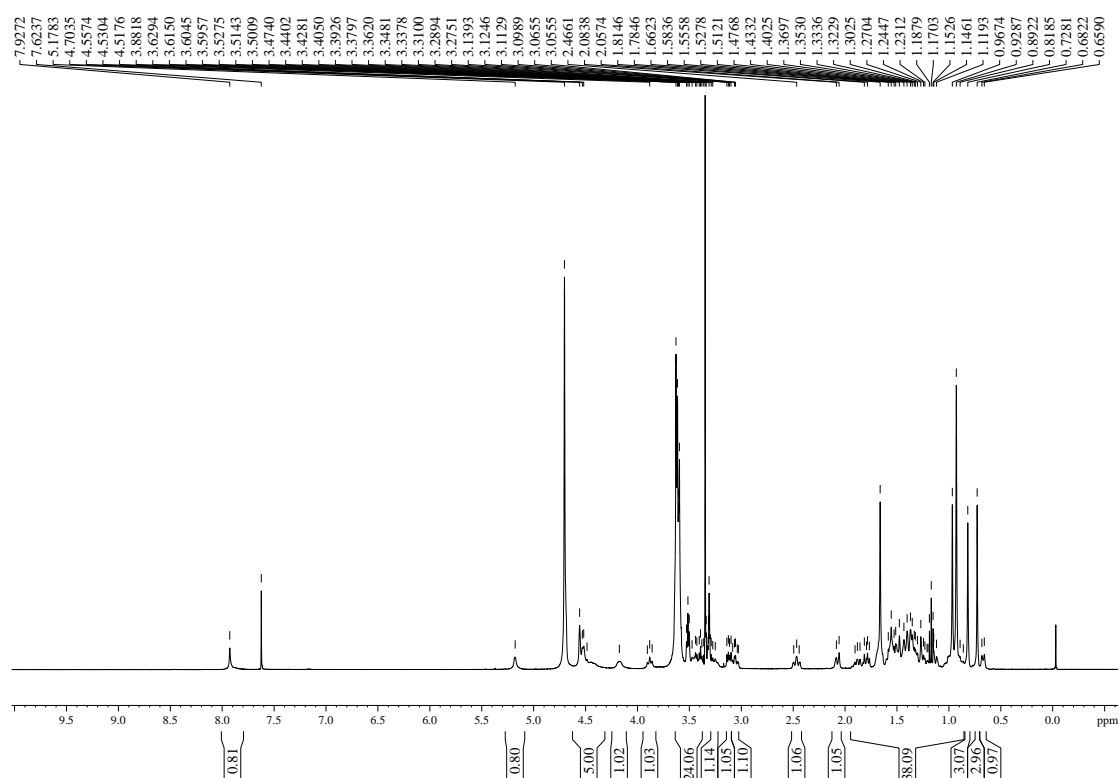
¹³C NMR of compound **82**



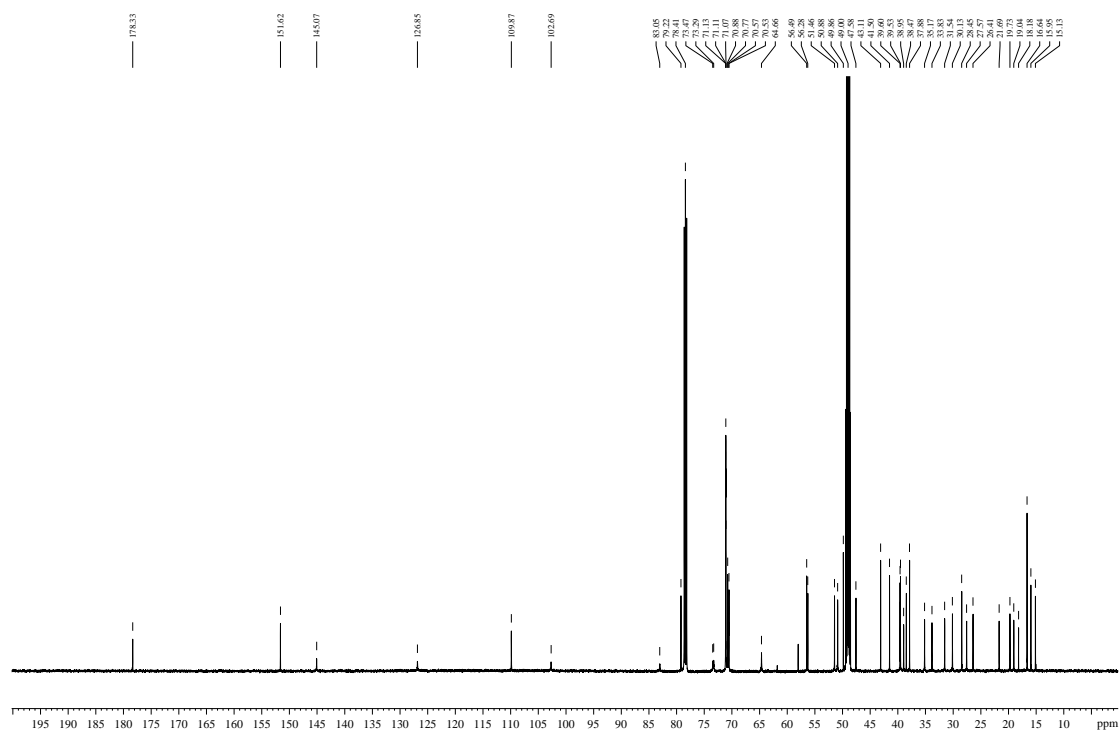
MALDI-TOF of compound **82**



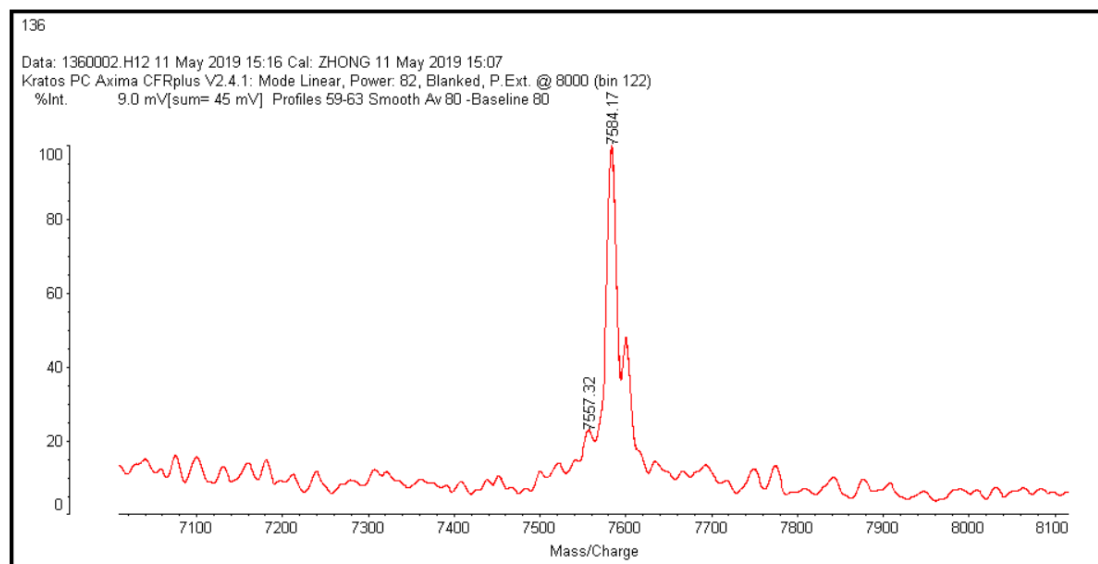
^1H NMR of compound **83**



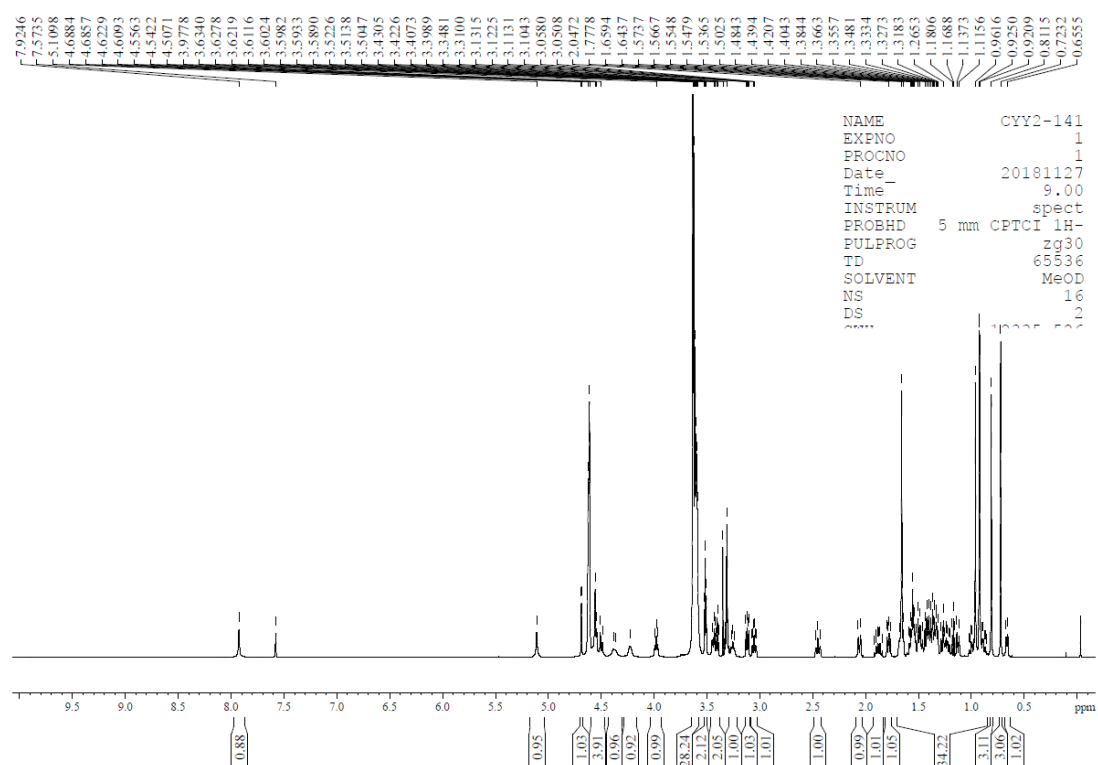
^{13}C NMR of compound **83**



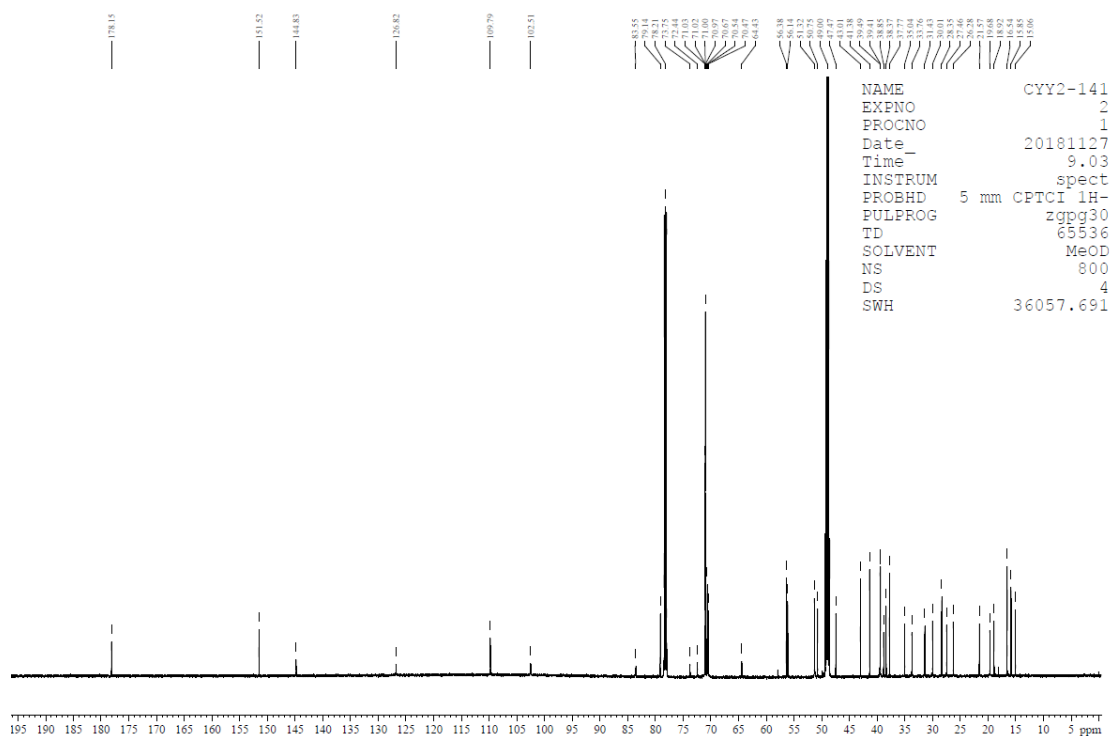
MALDI-TOF of compound **83**



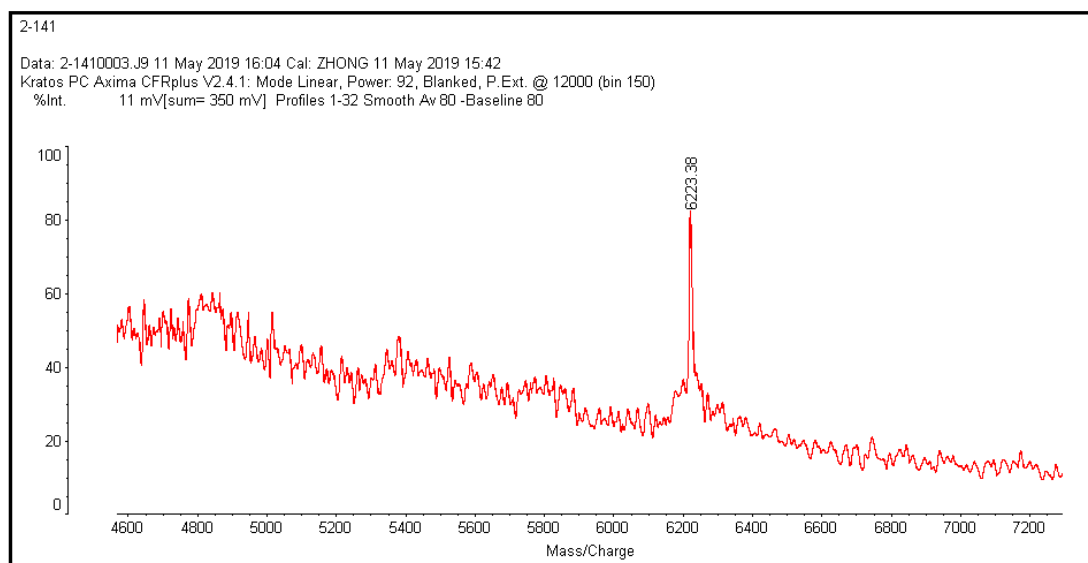
¹H NMR of compound 84



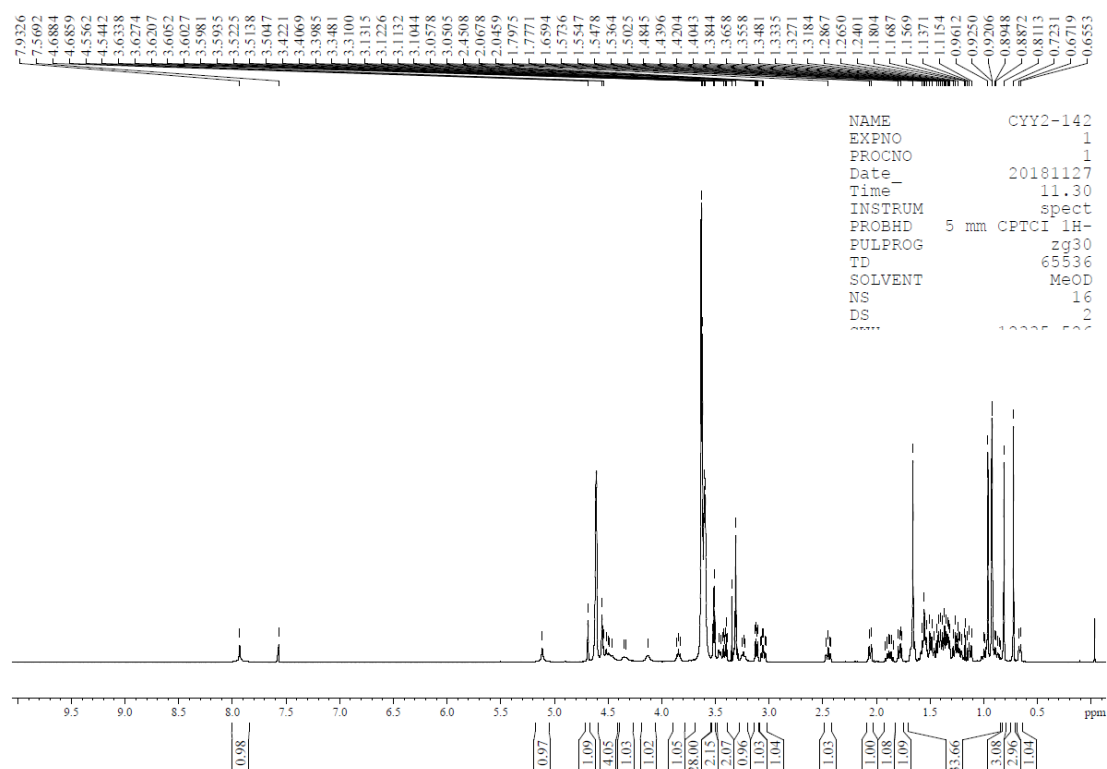
¹³C NMR of compound 84



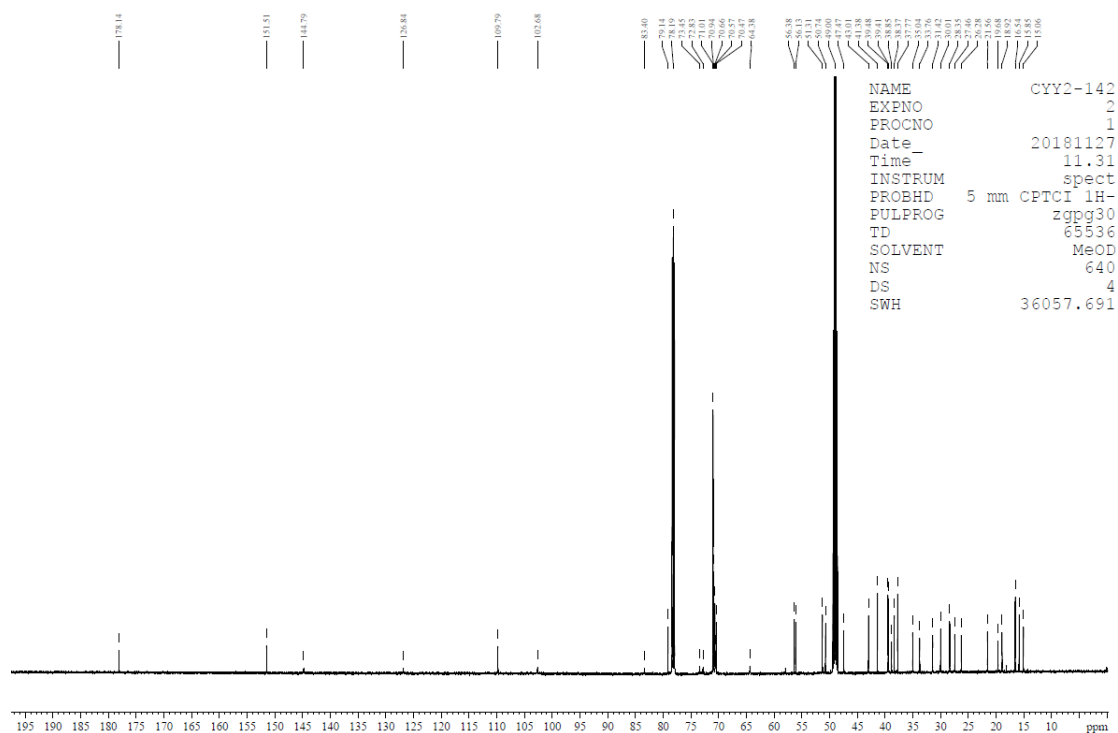
HRMS of compound **84**



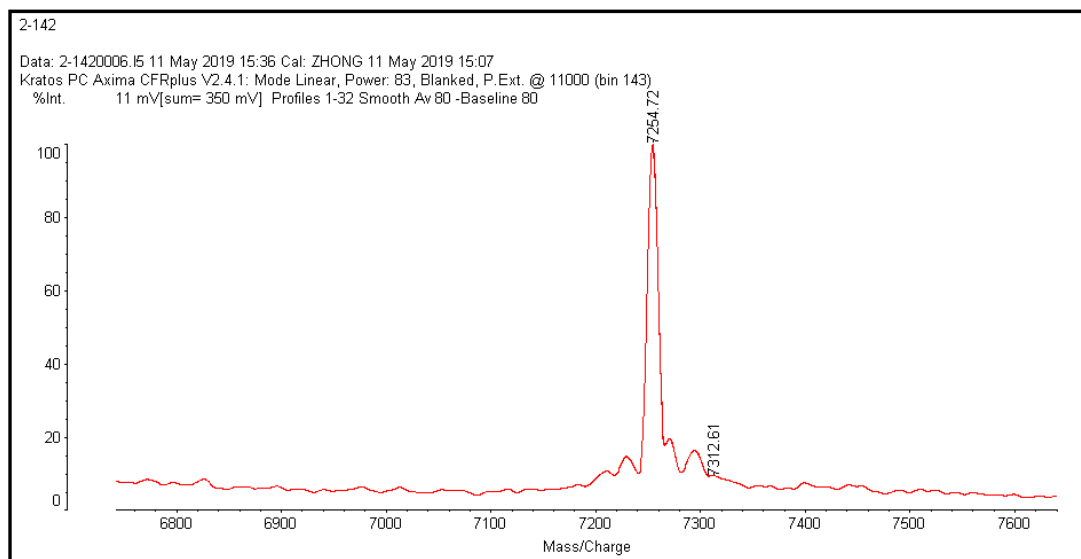
^1H NMR of compound **85**



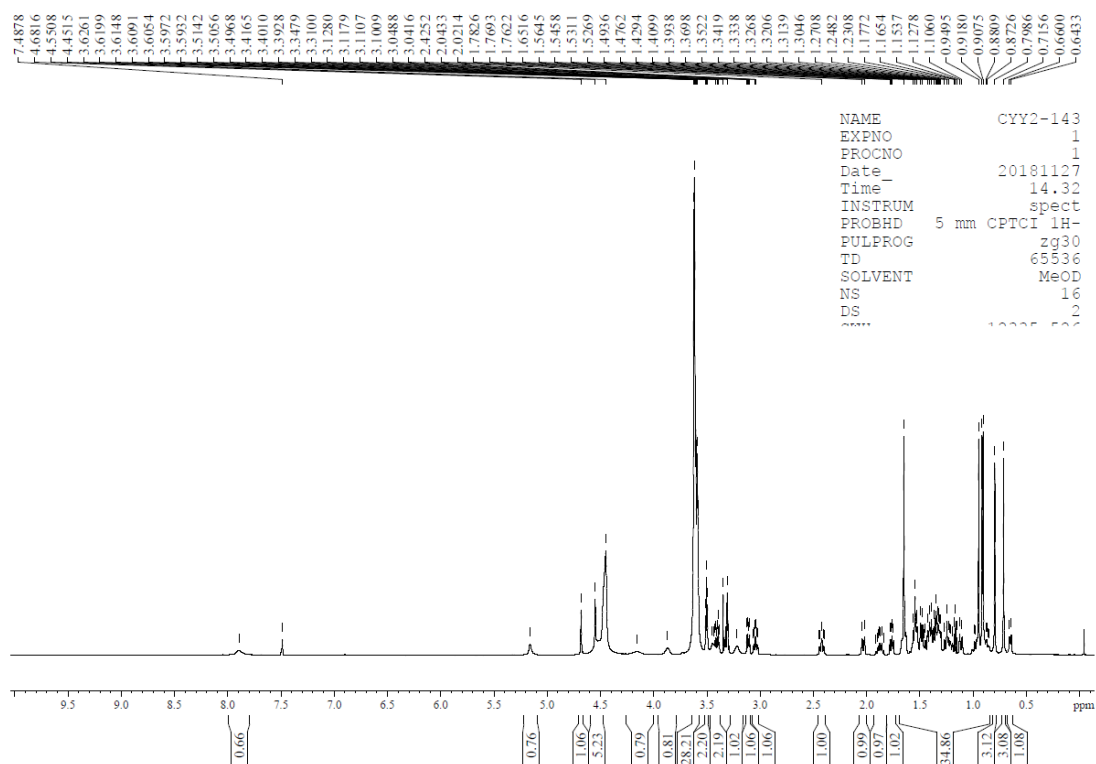
¹³C NMR of compound **85**



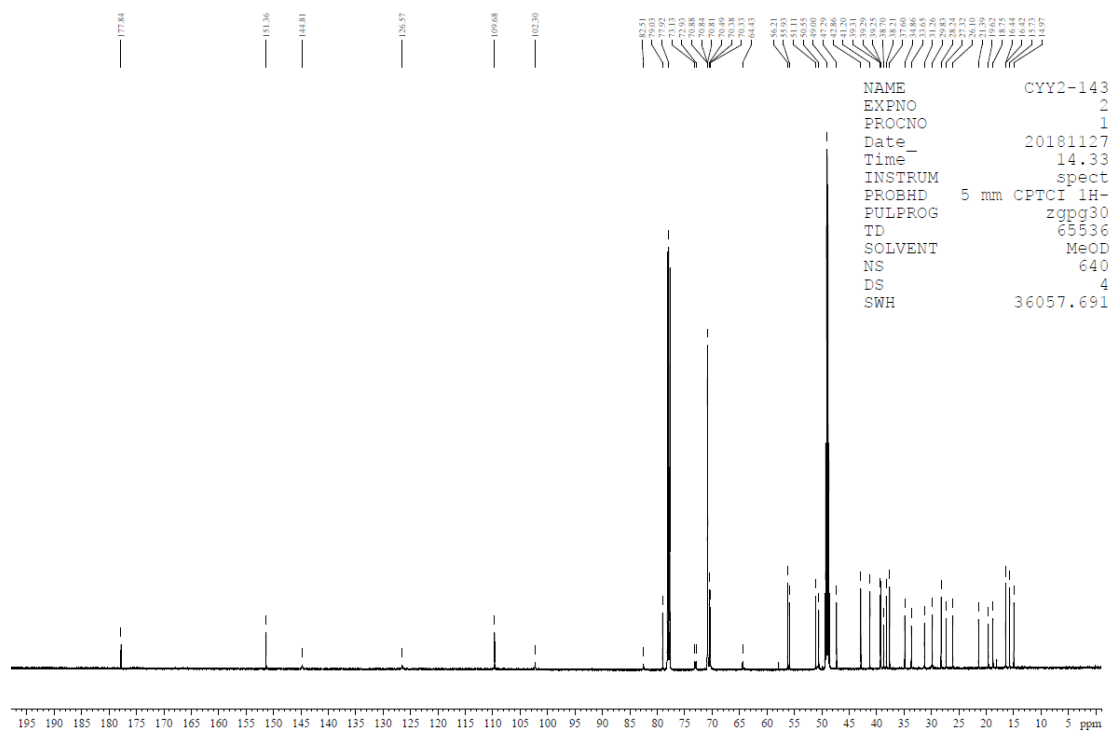
HRMS of compound **85**



¹H NMR of compound **86**



¹³C NMR of compound **86**



HRMS of compound **86**

